X Jubilee Conference

10th International Conference on Advanced Materials

BOOK OF ABSTRACTS

MINISTERUL CERCETĂRII,
INOVĂRII ȘI DIGITALIZĂRII

ROCAM 2024 | X Jubilee Conference
15 – 18 July, Bucharest, Romania
10th INTERNATIONAL CONFERENCE ON ADVANCED MATERIALS

History and Mission of ROCAM

The International Conference on Advanced Materials (ROCAM) is a prominent scientific event, held in Romania, dedicated to the field of advanced materials. Established to provide a platform for researchers, scientists, and industry professionals, ROCAM facilitates the sharing of the latest findings and developments in advanced materials.

The inaugural ROCAM conference took place in 1995, organized by several key institutions in the advanced materials landscape: the Romanian Academy, the Romanian Society of Materials Science and Crystal Growth, the National Institute of Materials Physics, and S.C. MATPUR S.A. The goal was to unite experts from various disciplines within materials science.

Over the years (1997, 2000, 2003, 2006, 2009, 2012, 2015, and 2017), the conference has grown in both size and scientific horizons, emerging as a significant scientific event at both regional and international levels. It has become one of the foremost venues and networking hubs, enabling the forging of solid collaborations between Romanian scientists and research institutions worldwide.

Now, celebrating its *10th edition*, ROCAM has evolved to cover crucial topics such as advanced nanomaterials, 2D materials, smart materials for high-tech applications, or biomaterials, all explored through an interdisciplinary approach that integrates physics, chemistry, various branches of engineering, and biology.

ROCAM aims to continue advancing research and development, bridging the gap between academic researchers, industry professionals, and stakeholders, and supporting the education and training of young researchers and students. These elements are crucial for fostering sustained progress in fundamental science, technological innovation, and the development of advanced materials.

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History of the National Institute of Materials Physics (NIMP)

Established in 1949, the Institute of Physics of the Romanian Academy was founded by Horia Hulubei, a distinguished scientist renowned for his ground-breaking contributions to various fields of physics, including Raman, X-rays, Compton, atomic, and nuclear physics. Hulubei earned his PhD in Paris under the tutelage of Nobel Prize laureates Pierre Curie and Maria Skłodowska-Curie.

In 1956, the Institute underwent a division resulting in the formation of two separate entities: the Institute of Atomic Physics (IFA) in Măgurele & the Bucharest Institute of Physics (IFB), the latter led by the Acad. Prof. Eugen Bădărău. E. Bădărău, a prominent professor from Sankt Petersburg and Cernăuți Universities, played a pivotal role in advancing the Romanian school of physics, particularly in the study of electrical discharges in gases and plasma.

Relocating to Măgurele in 1974, the Institute experienced further transformation in 1977 with the amalgamation of laboratories from IFB and IFA, forming the Institute of Physics and Technology of Materials. In 1996 it was officially rebranded the ***National Institute of Materials Physics (NIMP)*** following a national accreditation process, subsequently re-accredited in 2008 and 2016.

Throughout its history, NIMP has been home to distinguished physicists such as Acad. Eugen Bădărău, Acad. Radu Grigorovici, Acad. Ioan Iovitz Popescu, Acad. Margareta Giurgea, Acad. Rodica Mănăila, or Acad. Vladimir Țopa.

Over the past fifty years, NIMP has emerged as a leading research institution in Romania, investing over 35 million EUR in a new laboratory building equipped with state-of-the-art research facilities and the restoration of the historic Oteteleșanu Hall. Internationally, NIMP has played a significant role as one of the founders of the Central European Research Infrastructure (C-ERIC) and as an associated member of the Francophone University Agency (AUF). Additionally, it hosts a UNESCO category 2 centre – the Centre for Advanced Training and Research in Physics (CIFRA).

The mission of NIMP is to conduct cutting-edge research and advance innovation in materials science through the development of new materials and advanced technologies. By collaborating closely with research institutions and industrial stakeholders, NIMP aims to address key societal challenges. Additionally, NIMP is committed to providing education and training to the next generation of scientists from Romania and abroad.

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History of the Faculty of Physics at the University of Bucharest

The ***Faculty of Physics*** at the University of Bucharest has a rich history and is currently the largest among similar faculties in Romania. The University of Bucharest was founded in 1864 by a decree of Prince Alexandru Ioan Cuza of the Romanian Principalities. Initially, physics courses were offered within the Faculty of Sciences. As interest in physics grew, new administrative structures were established to accommodate this expansion.

In 1948, the Faculty of Mathematics and Physics was created from the Faculty of Sciences. In 1962, this faculty was further divided into the Faculty of Mechanics and Mathematics and the Faculty of Physics. In 1974, the Faculty of Physics relocated from Bucharest to a new campus in Măgurele, forming the National Platform of Physics in conjunction with the Central Institute of Physics.

Today, the Faculty of Physics at the University of Bucharest is organized into three departments, specializing in atomic and nuclear physics, condensed matter physics, biophysics, theoretical physics, lasers and photonics, and atmospheric and planetary physics.

The Faculty of Physics remains dedicated to academic excellence and scientific progress. It actively engages in outreach activities to promote science education and public understanding of physics and is a leading provider of qualified personnel for the Physics Institutes at Măgurele.

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MINISTERUL CERCETĂRII,
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PLENARY SPEAKERS

Klaus VON KLITZING

Nobel Prize for Physics in 1985

Monday, 15th of July 2024, 09:00 – 9:45

"The quantum revolution in metrology"

Klaus von Klitzing *was born in 1943 in Schroda. He received his PhD from the University of Würzburg in 1972. After research stays in England, USA and France he became a Professor at the Technical University in Munich in 1980. Between 1985 - 2018 he was director at the Max Planck Institute for Solid State Research in Stuttgart, Germany. He has been awarded the Nobel Prize in Physics in 1985 for the discovery of the Quantum Hall Effect. This quantum effect opened a new research field and plays a major role in metrology, not only as a resistance standard* $R_K=h/e^2$ *with the Planck constant h and the elementary charge e, but also in connection with the realization of a new SI system, based on fundamental constants.*

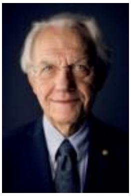
He has published more than 500 papers in the field of semiconductor quantum structures and received a large number of national and international awards. He holds 22 honorary degrees and is a foreign member of the National Academy of Sciences of the United States of America, the Russian Academy of Sciences, the Royal Society of London, the Chinese Academy of Sciences and the Pontifical Academy of Sciences.

Gérard Albert MOUROU

Nobel Prize for Physics in 2018

Monday, 15th of July 2024, 09:45 – 10:30

"Applications of ultra-short laser pulses in materials science"



Gérard Mourou *was born in Albertville, France. He studied physics at the University of Grenoble and then at the Université Pierre-et-Marie-Curie in Paris, where he earned his PhD in 1973. He later moved to the United States and became a professor at the University of Rochester, where he did his Nobel Prize awarded work along with Donna Strickland. He subsequently worked at the University of Michigan and the École Polytechnique in Paris. The sharp beams of laser light have given us new opportunities for deepening our knowledge about the world and shaping it. In 1985, Donna Strickland and Gérard Mourou succeeded in creating ultrashort high-intensity* *laser pulses without destroying the amplifying material. First they stretched the laser pulses in time to reduce their peak power, then amplified them, and finally compressed them. The intensity of the pulse then increases dramatically. Chirped pulse amplification has many uses, including corrective eye surgeries. He advanced laser science in Europe through his proposal of the Extreme Light Infrastructure, which consists of three facilities with extremely powerful lasers in the Czech Republic, Romania, and Hungary.*

Rodrigo MARTINS

Director of CENIMAT|i3N & CEMOP/UNINOVA,
President of European Academy of Sciences – EurASc

Tuesday, 16th of July 2024, 09:00 – 9:45

"Materials for eco-design strategies for an innovative industry"

Rodrigo Martins *was born in Nova Lisboa, Angola. He got in 1974 the Honours degree in Electronics Engineering, Telecommunications and applied Electronics by U. Luanda, Angola/Portugal. In 1977 he got the MSc degree in Semiconductor Materials, by the University of Dundee, Scotland, with a thesis entitled "Photoconductivity in P Doped and Undoped Amorphous Germanium" under supervision of Prof. W. Spear, 1977 Euro physicist award. In 1982 he obtained the Ph.D. in Energy conversion and Semiconductors, by New University of Lisbon, Portugal. PhD thesis title was "a-Si:H solar cells processing and characterization". In 1988 he got the Habilitation in Semiconductor Materials and Microelectronics, by New University of Lisbon, Portugal. Rodrigo Martins is now the President of the EurASc - European Academy of Sciences, Full Professor of Faculty of Sciences and Technology of New University of Lisbon in the field of Advanced Functional Materials and Microelectronics, Director of the Centre of Excellence in Microelectronics and Optoelectronics Processes of the Institute of New Technologies – CEMOP and Director of the Centre of Advanced Materials, CENIMAT. He is also President of the administration board of the Portuguese cluster in Advanced Materials (NANOMAT), member of the administration board of the Portuguese cluster on Batteries (BatPower), Chair of the European Committee Affairs of European Materials Research Society and Editor in Chief of the Journal Materials Discover, from Nature-Springer, member of the international advisory board of Advanced Electronics Materials. Rodrigo Martins published more than 1000 papers and has an h-index of 92.*

PLENARY SPEAKERS

Elvira FORTUNATO

Department of Materials Science of the Faculty of Science and Technology of the NOVA University of Lisbon

Tuesday, 16th of July 2024, 09:45 – 10:30

"From forest to electronic and biomedical applications"

***Elvira Fortunato**, Minister of Science, Technology and Higher Education of the government of Portugal, is a Professor at the Department of Materials Science of the Faculty of Science and Technology of the NOVA University of Lisbon. She has pioneered European research in transparent electronics using sustainable materials and environmentally friendly technologies. In 2008, in the 1st edition of the European Research Council (ERC) grants, she won an Advanced Grant with the INVISIBLE project, considered by the European Commission a success story. In the same year she demonstrated with his group the possibility of making the first paper transistor, starting a new field in the area of paper electronics. In 2018 she received the second Advanced Grant with the DIGISMART project. With more than 850 scientific publications, 58 patents conceived, Elvira Fortunato has received, in recent years, more than 30 international awards and distinctions for her work, including the decoration with the degree of Grand Officer of the Order of Prince Henry the Navigator, by the President of the Portuguese Republic in 2010; the Blaise Pascal Medal in 2016; the Czochralski Prize in 2017; the 2020 Pessoa Prize; the European Commission's Horizon Impact Award in 2020 with the INVISIBLE project; the Strait of Magellan Prize from the Government of Chile in 2020; the International Engineering Award in 2021; the Human Rights Award by the Assembly of the Republic in 2021; The Materials Frontiers Award 2022, given by IUMRS and Chinese-MRS; the SPM career recognition award 2022. Moreover, her work in the area of green electronics and paper electronics has been considered one of the 20 best ever innovators in Europe. She is an elected member of the Academy of Engineering, the European Academy of Sciences, the Lisbon Academy of Sciences and the Academia Europaea. She was a member of the Board of Trustees of the Luso-American Development Foundation between 2014 and 2021. She was a member of the High-Level Group for the European Commission's Scientific Advice Mechanism between 2015 and 2020. She has coordinated several national and international* *projects, including her pioneering activity at Universidade Nova de Lisboa in the area of equal opportunities through the SPEAR project, a European platform for the support and implementation of plans for gender equality in higher education institutions.*

Rafal E. DUNIN-BORKOWSKI

Institute for Microstructure Research and the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons in Forschungszentrum Jülich, Germany

Tuesday, 16th of July 2024, 14:30 – 15:15

"Exploring the nano-world with electrons"

Rafal Dunin-Borkowski *is Director of the Institute for Microstructure Research and the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons in Forschungszentrum Jülich, Germany. His Ph.D. (1990-1994) was carried out in the Department of Materials Science and Metallurgy in the University of Cambridge. After working as, a postdoctoral research scientist in the University of Cambridge, Arizona State University and Oxford University, between 2000 and 2006 he held a Royal Society University Research Fellowship in the University of Cambridge. Between 2007 and 2010, he led the establishment of the Center for Electron Nanoscopy in the Technical University of Denmark. He specializes in the characterization of magnetic and electronic materials at the highest spatial resolution using advanced transmission electron microscopy techniques, including aberration-corrected high-resolution transmission electron microscopy and off-axis electron holography. In 2009 he was awarded the Ernst Ruska Prize of the German Society for Electron Microscopy. In 2012, 2017 and 2019 he was awarded Advanced, Proof of Concept and Synergy Grants by the European Research Council.*

PLENARY SPEAKERS

Paolo FORNASIERO

University of Trieste, Italy

Tuesday, 16th of July 2024, 15:15 – 16:00

"Sustainable processes: Producing better and more with less"

Paolo Fornasiero *is Professor of Inorganic Chemistry at the University of Trieste. His scientific interests are in the field of inorganic chemistry, with attention to the design and development of multi-functional nano-systems and their advanced applications in energy related processes and environmental heterogeneous catalysis. Paolo Fornasiero has published more than 300 research articles, 19 book chapters, and holds 4 patents. Since 2022 he is member of the Academia Europaea and from 2021 he is member of the European Academy of Sciences. He received various awards including the 2005 Nasini Medal, the 2013 Chiusoli Medal and the Malatesta award from the Italian Chemical Society, the 2016 Heinz Heinemann Award from the International Association of Catalysis Societies.*

Thomas SCHROEDER

Director IKZ Berlin

Wednesday, 17th of July 2024, 09:00 – 09:45

"IKZ for EU: Latest R & D trends on synthesis & applications of crystalline materials"

Thomas Schroeder *is Scientific Director of the Leibniz-Institut für Kristallzüchtung (IKZ) in Berlin and Professor in Crystal Growth at the Institute of Physics of the Humboldt University zu Berlin. His R&D interests are focused on innovations in crystalline materials (numerical simulation, plant engineering, growth techniques etc.) and innovations by crystalline materials (crystal preparation techniques, applications of crystalline materials in electronics and photonics etc.). Since 2004, Thomas Schroeder worked in the Materials Science Department of the Leibniz-Institute for innovative Microelectronics (IHP) in Frankfurt (Oder) where he became department head in 2009 and full professor in semiconductor physics at the Technical University of Brandenburg in Cottbus in 2012. The PhD thesis was carried out from 1998 to 2001 at the Fritz-Haber-Institute* *of the Max-Planck Society in Berlin on catalytic processes. He received a diploma degree in Chemistry in 1996 and a diploma degree in Physics in 1998 from the University of Tübingen. He passed several research and PostDoc stays in European institutes in Italy, Spain and France.*

Marin ALEXE

Department of Physics, University of Warwick, Coventry UK

Wednesday, 17th of July 2024, 09:45 – 10:30

"Symmetry breaking and novel photovoltaic effects in oxide perovskites"

*Professor **Marin Alexe** has been appointed as Chair of Functional Materials at the University of Warwick after spending about 18 years at the Max Planck Institute of Microstructure Physics-Halle, Germany (1996-2013) and about 10 years at the National Institute of Materials Physics, Romania (1987-1996). He has received the PhD degree from the Institute of Atomic Physics Bucharest in 1995. His research interest is physics and engineering of ferroelectrics, complex oxide thin films for information technology and integration of functional materials for oxide electronics. He has published more than 325 papers and 2 books. In the last five years he has given more than 30 invited talks and lectures at international meeting and conferences. He was recently awarded Wolfson Research Merit and Theo Murphy "Blue Sky" Awards of the Royal Society as well as Alexander von Humboldt research Award.*

Adrian M. IONESCU

EPFL Lausanne, Switzerland

Thursday, 18th of July 2024, 09:00 – 09:45

"Emerging nanoelectronics and artificial intelligence: Convergence, challenges and opportunities"

***Adrian M. Ionescu** is a Full Professor at Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland. He received the BS & MS in Electronics and Telecommunications in 1989 from University 'Politehnica' Bucharest, Romania. He holds two PhDs: in Microelectronics, from UPB (1994) and in Physics of semiconductors from National Polytechnic Institute Grenoble (1997). He is director of Nanoelectronic Devices Laboratory of EPFL, Switzerland. His group pioneered novel device concepts and technologies for energy efficient Edge Artificial Intelligence and Internet of Things applications. He published more than 600* *articles. He is recipient of IBM Faculty Award 2013 and of André Blondel Medal 2009. In 2015 he was elected member of Swiss Academy of Technical Sciences. He received an ERC Advanced Grant in 2016, a ERC Synergy grant in 2023 and the EDL IEEE George Smith Award in 2017. He is an IEEE Fellow and he served as Editor of IEEE TED and as member of PUB committee of EDS. He is a member of the Editorial Board of Proceedings of IEEE. Recently, he received the prestigious 2024 IEEE Cledo Brunetti field Award.*

Nicolae BARSAN

Institute of Physical and Theoretical Chemistry,
University of Tübingen, Germany

Thursday, 18th of July 2024, 09:45 – 10:30

"Gas sensing with semiconducting metal oxides: The interplay between chemistry, physics and engineering"

Nicolae Barsan *received his diploma in Physics from the Faculty of Physics of the Bucharest University in 1982. In 1993 his received his Ph.D. in Solid State Physics from the Institute of Atomic Physics, Bucharest, Romania. Since 1995 he has been a senior researcher at the Institute of Physical Chemistry of the University of Tuebingen, where he and Udo Weimar lead the Gas Sensors Group. Dr Barsan's research focuses on the understanding and application of surface interactions of materials with gases. At the Institute of Physical Chemistry, he advanced his interest in the basic understanding of sensing with metal oxide pioneering the operando approach that employs a host of spectroscopic and phenomenological characterization techniques, applied in sensor operation conditions. On the technology side, he invented the hybrid microsensor production technology combining pre-processed powders-based sensing layers and micromachined Si transducers; to date, more than 50 million devices, of the type invented by Dr. Barsan, were commercialized by AppliedSensors (currently owned by AMS, Austria). In 2006 he co-founded AO Action, which is a Steinbeis Transfer Centre working in the exploitation of advanced sensing technologies. The Centre provides commercial services to private clients. Dr. Barsan is one of the two directors and currently runs 3 projects for industrial customers.*

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SCIENTIFIC PROGRAM of ROCAM 2024

Section 1 (S1): *Bulk Crystals, Ceramics, and Composites*
Section 2 (S2): *Thin Films, 2D Systems, and Nanostructures*
Section 3 (S3): *Advanced Characterization Methods*
Section 4 (S4): *Applications of Advanced Functional Materials*

Venue Location: J.W. MARRIOTT BUCHAREST GRAND HOTEL
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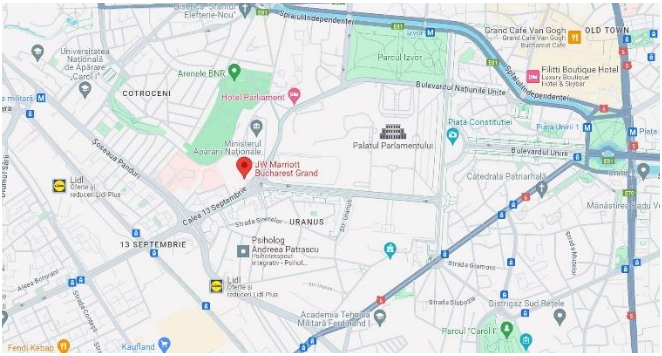

Day 1, Monday, 15th of July 2024

Lobby of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
07:00 09:00	**Registration**						
Grand Ball Room AB – **PLENARY LECTURES (PL) SESSION** Chair: **Lucian PINTILIE**							
09:00 09:45	**PL1: Klaus VON KLITZING – "The quantum revolution in metrology"**						
09:45 10:30	**PL2: Gérard Albert MOUROU – "Applications of ultra-short laser pulses in materials science"** (*presented by Dr. Gabriel P. Bleotu on behalf of Prof. Mourou*)						
Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
10:30 11:00	**Coffee/Tea Break**						
INVITED LECTURES (IL) & ORAL PRESENTATIONS (OP) SESSIONS							
Brasov Hall – **S1** Chair: **Traian DUMITRICA**		Grand Ball Room A – **S2** Chair: **Stela CĂNULESCU**		Craiova Hall – **S3** Chair: **Marco BELEGGIA**		Grand Ball Room B – **S4** Chair: **Anatoli SERGHEI**	
11:00 11:30	**S1-IL1: L. MITOSERIU** "Ag-BaTiO$_3$ CERMETs with tunable meta-composites properties"	11:00 11:30	**S2-IL1: F. SÁNCHEZ** "Disentangling stress and strain effects in ferroelectric HfO$_2$"	11:00 11:30	**S3-IL1: B. SHIN** "Carrier-resolved photo-Hall effect"	11:00 11:30	**S4-IL1: T. GRANZOW** "Able to take the heat? – Ferroelectric oxides in electrocaloric applications"
11:30 12:00	**S1-IL2: A.C. IANCULESCU** "Multifunctional (Ba,Sr)TiO$_3$ systems: From nanopowders to bulk ceramics"	11:30 12:00	**S2-IL2: A. DIMOULAS** "Hafnia-based ferroelectric field effect memristor synapses epitaxially grown on silicon"	11:30 12:00	**S3-IL2: W. BETZ** "Analysis of buried interfaces for device technology by soft and hard X-ray photoemission"	11:30 12:00	**S4-IL2: A. CRUNTEANU** "Phase change materials for reconfigurable terahertz (meta) devices: integration and challenges"
12:00 12:20	**S1-OP1: R.S. STIRBU** "Local *vs.* macroscopic	12:00 12:20	**S2-OP1: C. BESLEAGA** "Oxygen vacancies and	12:00 12:20	**S3-OP1: C. ROMANITAN**	12:00 12:20	**S4-OP1: A.G. BONI** "Strategies for achieving

	properties of porous BaTiO$_3$ ceramics based on 3D reconstructed ceramic microstructure”		applied electrical field conditioning of polar phase in hafnia nanocrystals”		“Strain analysis in vanadium oxide thin films by Rietveld refinement”		steady-state negative capacitance in ferroelectric multilayered structures”
12:20 12:40	**S1-OP2: L. ROMAGNOLI** “A convenient synthesis of BaZrS$_3$, BaHfS$_3$ and their solid solutions at moderate temperature”	12:20 12:40	**S2-OP2: V. MUSAT** “Some contributions to metal oxide-based multifunctional hybrid thin films for transparent and flexible electronics by bottom-up approach”	12:20 12:40	**S3-OP2: M.I. ZAI** “X-Ray diffraction study of threading dislocations in epitaxial gallium nitride thin films grown by molecular beam epitaxy”	12:20 12:40	**S4-OP2: C. JALBA** “High throughput graphene production via intercalation-expansion method”
12:40 13:00	**S1-OP3: A. TILIAKOS** “Non-Arrhenius anomalies and large polaron tunneling mechanisms in NaSICON superionic ceramic conductors”	12:40 13:00	**S2-OP3: K. UNGEHEUER** “Thin film cupric oxide as absorbing layer for solar cells in space applications”	12:40 13:00	**S3-OP3: L. SOCACIU-SIEBERT** “NAP-XPS instrumentation and applications”	12:40 13:00	**S4-OP3: O.A. RADUCU** “Biosynthesized gold nanoparticles: Tunable thermo-plasmonic nanogenerators from visible region to NIR I and II Biological Windows”
Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
13:00 14:30	**Lunch**						
Brasov Hall – S1 Chair: **Liliana MITOSERIU**				Craiova Hall – S3 Chair: **Byungha SHIN**		Grand Ball Room A– S4 Chair: **Mihaela MATACHE**	
14:30 15:00	**S1-IL3: T. DUMITRICA** “Enhancing the mechanical properties of carbon nanotube materials through computationally guided engineering of interactions between	14:30 15:00		14:30 14:50	**S3-OP4: J. DE LA FIGUERA** “Observing barium oxide on W(110) by low-energy, thermionic and photoemission electron microscopy”	14:30 15:00	**S4-IL3: M. BIANCHI** “Micro/nanopatterning of conductive polymers for advanced biointerfaces”

	fibers at the mesoscale level”						
15:00 15:20	**S1-OP4: A.M. BADEA (IONESCU)** “Vortex dynamics in some representative Iron-based superconducting single crystals”	15:00 15:20		14:50 15:10	**S3-OP5: L.E. BORCAN** “Surface magnetism of platinum (001) and strontium titanate (001) investigated by spin-resolved photoelectron spectroscopy”	15:00 15:20	**S4-OP4: C.P. CONSTANTIN** “Double electron donor-embedded polymers for energy-efficient smart windows”
15:20 15:40	**S1-OP5: S. POLOSAN** “Morphology and structural properties of M-hexaferrite”	15:20 15:40		15:10 15:30	**S3-OP6: A.E. BOCIRNEA** “The effects of ultrahigh vacuum treatments on SnSe flakes transferred on naturally oxidized Si wafers”	15:20 15:40	**S4-OP5: A.C. SERGENTU** “*In vitro* hyperthermia with iron oxide magnetic nanoparticles”
15:40 16:00	**S1-OP6: C.M. TEODORESCU** “A revised theory of band ferromagnetism”	15:40 16:00		15:30 15:50	**S3-OP7: M. HUSANU** “Intrinsic electronic structure of oxide surfaces and interfaces from angle resolved photoelectron spectroscopy”	15:40 16:00	**S4-OP6: V. KUNCSER** “VO$_2$ based thermochromic coatings for smart window applications”
Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
16:00 16:30	**Coffee/Tea Break**						
16:30 18:00	**POSTER PRESENTATION (PP) SESSIONS of SECTIONS 1 & 2** ***Commission for Best Poster Awards:*** **Torsten GRANZOW, Nicolae SPALATU, Valérie DEMANGE**						
	S1-PP1: M. HUSANU; “Al-doped SrTiO$_3$ photocatalyst with increased performance”.						
	S1-PP2: M. BOTEA; “Bulk graded (Ba,Sr)TiO$_3$ structures with enhanced thermal stability”.						
	S1-PP3: L. NEDELCU; “Thermal drift in Ba$_{1-x}$Sr$_x$TiO$_3$/polyethylene composites studied by broad-band dielectric spectroscopy”.						

	S1-PP4: O. BABATUNDE & **E. IMORU**; **“**Morphological and phase examination of mullite based ceramics developed using synthesized amorphous silica from rice husk ash**”.**
	S1-PP5: M.C. CIOANGHER; **“**Sr and Ga doped barium titanate piezoceramics for osteogenic applications**”.**
	S1-PP6: M. BOJAN & **C. UDREA**; **“**Terahertz-Time-Domain Spectroscopy for heavy metals detection in soil**”.**
	S1-PP7: C.S. FLORICA; **“**Composites based on polydiphenylamine and multi-wall carbon nanotubes functionalization with carboxylic acid groups for applications in energy storage**”.**
	S1-PP8: T. BURLANESCU; **“**Composites containing poly(vinylchloride) for applications as SERS supports and membranes used in filtration processes**”.**
	S2-PP1: L.D. FILIP; **“**Investigation of the insulator layer role in polarization direction stability in multilayered heterostructures**”.**
	S2-PP2: L.M. BALESCU; **“**Wurtzite III-V materials for ferroelectric component in heterostructures**”.**
	S2-PP3: A.C. IANCU; **“**Swinging molecular adsorption of carbon monoxide on ferroelectric BaTiO$_3$(001)**”.**
	S2-PP4: C.F. CHIRILA; **“**Obtaining and tailoring electrical properties of epitaxial PZT thin films by different doping**”.**
	S2-PP5: C. ROTARESCU; **“**The effect of magnetoelastic anisotropy on the magnetization processes in amorphous nanowires**”.**
	S2-PP6: C.C. NEGRILA; **“**Structural and electronic properties of HfO$_2$ thin layers deposited on III-V semiconductor surfaces**”.**
	S2-PP7: I. DASCALESCU; **“**Hydrogenated GeSn films for short-wave infrared detection**”.**
	S2-PP8: V. MIHALACHE; **“**Exchange bias effect in ZnFe$_2$O$_4$(FIM)-FeO(AFM)-ZnO & ZnFeO(DMS)–FeO(AFM) nanocomposite systems**”.**
	S2-PP9: C. GHEMES; **“**Improvement of the tunnel magnetoresistance – based sensor by optimizing the deposition conditions**”.**
	S2-PP10: H. POPOVA; **“**Step meandering on vicinal surfaces: Crystal growth modeling based on cellular automata**”.**
	S2-PP11: M. TAMIN; **“**Synthesis and characterization of kesterite thin films Cu$_2$ZnSnS$_4$ solar cells with Ag substitution**”.**
	S2-PP12: A.G. NICULESCU; **“**3D-printed microfluidic devices for magnetic nano and microparticle synthesis of use in environmental applications**”.**
	S2-PP13: D.I. TUDORACHE; “Cross-flow 3D microfluidic device for aerogel nanocomposites synthesis”.
	S2-PP14: M.M. APOSTOL; **“**Growth graphene by chemical vapor deposition for electronic devices**”.**
	S2-PP15: C. ROMANITAN; **“**Dependence of La-doped ZnO nanocomposite properties of dopant concentration for semiconductor materials fabricated by electrospinning calcination method**”.**
	S2-PP16: A. SERGHEI; **“**Investigations of attograms and zeptograms of matter under extremely high electric fields**”.**
	S2-PP17: R. ALEKBEROV; **“**X-ray diffraction and Raman scattering of PbSe(S) thin films**”.**
	S2-PP18: F. GHERENDI; **“**In$_2$O$_3$ and ZnO thin film paper transistors fabricated by pulsed electron beam deposition**”.**
	S2-PP19: M. NISTOR; **“**How far oxygen deficiency can be driven in indium oxide thin films grown by pulsed electron beam

	deposition?**”.**
	S2-PP20: D.C. NASTAC; **“**Investigation of the electrospinning parameters on the manufacture of PVDF nanofibers**”.**
	S2-PP21: S. NISTOR; **“**Amyloid beta improved surfaces for development of biomedical applications**”.**
	S2-PP22: I. ANTOHE; **“**Synthesis of a highly sensitive NH_3 gas detection sensor through Co-doped ZnO thin-film using SILAR technique**”.**
	S2-PP23: M.I. ZAI; **“**Density functional theory computational study of the superconducting properties of palladium hydride systems**”.**
	S2-PP24: A.M. IAMANDI; **“**Exploring the generation of metal nanoparticles through laser ablation in liquid media**”.**
	S2-PP25: A. EL KANOUNY; **“**The influence of duty cycle on structural and optical properties of Tin Selenide thin films prepared by pulsed electrodeposition**”.**
	S2-PP26: A. CRIVEANU; **“**Studies regarding the optimization of the dispersion process of iron oxide nanoparticles synthesized by laser pyrolysis**”.**
	S2-PP27: F. DUMITRACHE; **“**Spectacular dispersibility of oxide nanoparticles synthesized by laser pyrolysis with isopropanol vapors as sensitizer**”.**
	S2-PP28: E. PETRE; **“**Exciton-photon coupling in ZnO optical microcavities fabricated by pulse laser deposition**”.**
	S2-PP29: F.I. CEARĂ & **M. ZAMFIRESCU**; **“**Design and characterization of integrated optics fabricated by two-photon polymerization**”.**
	S2-PP30: R. SAYED; **“**Effect of doping on the structural and optical properties of Co-doped ZnO thin films by electrodeposition method**”.**
	S2-PP31: S. SAADAOUI; **“**Study of optical and structural properties of mixed halides (I, Cl) of methylammonium-lead perovskite by spin-coating method for photovoltaic application**”.**
	S2-PP32: V. STANCU; **“**Growth and functionality of Cu_2ZnSnS_4 (CZTS) films: From nanoparticle ink to inorganic solar cells**”.**
	S2-PP33: L. TRUPINA; **“**Growth and characterization of vanadium dioxide thin films prepared by reactive-RF sputtering**”.**
	S2-PP34: L. PINTILIE; **“**Polarization switching triggered by charge injection: possible universal switching mechanism in ferroelectric thin films**”.**
	S2-PP35: S. HILGERS; **“**Exploring the structural and chemical composition of antimony monolayer on Ag(110)**”.**
	S2-PP36: I. STAVARACHE; **“**2D-MoS_2 selectively grown on Mo patterned substrates for photosensitive field effect transistor**”.**

Day 2, Tuesday, 16th of July 2024

Lobby of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
08:00 09:00	**Registration**						
Grand Ball Room AB – **PLENARY LECTURES (PL) SESSION** Chair: **Lucian PINTILIE**							
09:00 09:45	**PL3: Rodrigo MARTINS – “Materials for eco-design strategies for an innovative industry”**						
09:45 10:30	**PL4: Elvira FORTUNATO – “From forest to electronic and biomedical applications”**						
Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
10:30 11:00	**Coffee/Tea Break**						
INVITED LECTURES (IL) & ORAL PRESENTATIONS (OP) SESSIONS							
Brasov Hall – S1 Chair: **Adelina IANCULESCU**		Grand Ball Room A – S2 Chair: **Athanasios DIMOULAS**		Craiova Hall – S3 Chair: **Beata KARDYNAL**		Grand Ball Room B – S4 Chair: **Aurelian CRUNTEANU**	
11:00 11:20	**S1-OP7: N. DEMIRKOL** “Ternary hydroxyapatite-titania-graphene biocomposites produced by green process and their bioactivity behavior”	11:00 11:30	**S2-IL3: S. CANULESCU** “Unveiling nonlinear optical and electrical responses in molybdenum disulfide: A journey through 2D materials and beyond”	11:00 11:30	**S3-IL3: M. BELEGGIA** “Design, fabrication and characterization of adaptive electron-optical devices for beam shaping”	11:00 11:30	**S4-IL4: Z. JEHL LI-KAO** “From stagnation to success: Recent breakthroughs in kesterite solar cell technology for indoor Photovoltaics”
11:20 11:40	**S1-OP8: D.A. PIKULSKI** “Cu-Zr-Al metallic glass matrix composites with in-situ precipitated phase reinforcement”	11:30 12:00	**S2-IL4: N. SPALATU** “Towards developing emerging antimony and bismuth-based chalcogenide for next generation, Earth abundant photovoltaics”	11:30 12:00	**S3-IL4: M. KREMER** “X-ray diffraction for battery analysis: Modern challenges and modern solutions”	11:30 12:00	**S4-IL5: M. MATACHE** “Photo-sensitive azo-based small molecule switches”

11:40 12:00	**S1-OP9: M. STEFAN** "Composite photocatalysts based on carbon structure and semiconductors obtained by recycling electronic wastes"	12:00 12:20	**S2-OP4: A. STROPPA** "Chiral multiferroicity in two-dimensional hybrid organic-inorganic perovskites"	12:00 12:20	**S3-OP8: B. BORCA** "Advanced method for amino acid recognition within peptide sequences"	12:00 12:20	**S4-OP7: O. EL KHOUJA** "Synthesis, characterization and optoelectronic applicability of Sb_2S_3 thin films for enhanced solar energy conversion"
12:00 12:20	**S1-OP10: M. ENCULESCU** "Fabrication and characterization of sponge-like PDMS composites"	12:20 12:40	**S2-OP5: M.I. BELCIU & A. VELEA** "Prediction of glass formation ability in chalcogenides using machine learning algorithms"	12:20 12:40	**S3-OP9: R. DOBRE** "Momentum estimation of charged particles registered in a nuclear emulsion detector within the DsTau(NA65) experiment"	12:20 12:40	**S4-OP8: A.G. TOMULESCU** "Mitigating the toxicity during perovskite solar cell fabrication"
12:20 12:40	**S1-OP11: C. SECU** "Rare-earth doped GdF_3/$LiGdF_4$ nanocrystals in silica glassy nanocomposites: crystalline phase tuning and luminescence properties"	12:40 13:00	**S2-OP6: A.M. FLOREA (RADUTA)** "Physical properties of submicrometric RF-sputtered CdTe thin films for photovoltaic applications"	12:40 13:00	**S3-OP10: M. ADELMARK** "Fabrication of a thin-film adaptive electrostatic phase plate"	12:40 13:00	**S4-OP9: E. ALEMDAR YILMAZ** "Optical, electrochemical and photovoltaic properties of side chain effects on BDT and TPD-containing polymers"
12:40 13:00	**S1-OP12: M. GALATANU** "Improved thermo-physical and mechanical properties of Tungsten with dispersed nanometric ZrC particles processed by SPS and a subsequent thermo-mechanical treatment"						

Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL	
13:00 14:30	**Lunch**
Grand Ball Room AB – **PLENARY LECTURES (PL) SESSION** Chair: **Lucian PINTILIE**	
14:30 15:15	**PL5: Rafal E. DUNIN-BORKOWSKI – "Exploring the nano-world with electrons"**
15:15 16:00	**PL6: Paolo FORNASIERO – "Sustainable processes: Producing better and more with less"**
Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL	
16:00 16:30	**Coffee/Tea Break**
16:30 18:00	**POSTER PRESENTATION (PP) SESSIONS of SECTIONS 3 & 4** ***Commission for Best Poster Awards:* Torsten GRANZOW, Nicolae SPALATU, Valérie DEMANGE**
	S3-PP1: M.C. ISTRATE; **"**New deposition method for achieving ferroelectric orthorhombic ZrO_2**".**
	S3-PP2: A.T. NEAGU; **"**Production of a few alpha pairs in interactions of light nuclei with nuclear emulsion**".**
	S3-PP3: C. RADU & **A.C. KUNCSER**; **"**From electron tomography to magnetic properties using micromagnetic simulations**".**
	S3-PP4: I.C. CIOBOTARU; **"**Structural and photophysical properties of antimony hybrid perovskites for organic light emitting diode applications**".**
	S3-PP5: P. POPOV & **M.E. MIHAILOV**; **"**Exploring underwater objects through magnetometry techniques – Methods and assessment**".**
	S3-PP6: A. SIMEDRU; **"**Effects of several accelerators` working mechanisms on Portland cement concrete structure and mechanical properties**".**
	S3-PP7: A.E. MINUTI; **"**Scanning electron microscopy as pathway to study on the adherence of nanomaterials on cells**".**
	S3-PP8: S.A. YEHIA-ALEXE; **"**Hydrogen isotopes released from beryllium layer by Laser Induced Desorption and Laser Induced Ablation**".**
	S4-PP1: C. MARCULESCU; **"**Improving the conductivity of FETs based on carbon nanomaterials by decorating the nanomaterial surface with gold nanoparticles**".**
	S4-PP2: M. PIEKARCZYK; **"**Advancements in smart material systems for micro 4D printing: fabrication, actuation and characterization**".**

	S4-PP3: L.N. LEONAT; **“**Study of protonated diamines for the improvement of the morpho-structural characteristics of hybrid halide perovskite films**”.**
	S4-PP4: O. CRACIUNESCU; **“**Evaluation of the viability of 3D stem cell spheroids in a hydrogel matrix for dental tissue regeneration**”.**
	S4-PP5: D. GHERCA; **“**Entropy-engineered spinel-type mixed oxides for photocatalytic oxygen evolution reaction**”.**
	S4-PP6: I. ZGURA; **“**Photocatalytic activity of composite materials based on ZnO and CuO commercial powders**”.**
	S4-PP7: E. CHIRIAC; **“**Development and optimization of a microfluidic device for exosome filtration**”.**
	S4-PP8: A.G. MIREA; **“**Low metal loading supported on MAX Phases for selective hydrogenation of cinnamaldehyde**”.**
	S4-PP9: I. SPINU; **“**Transport mechanisms in IGZO memristor**”.**
	S4-PP10: M.I. CHIRICA; **“**2D $Ti_3C_2T_x$ MXene as electrode on all oxide capacitors deposited by spray coating method**”.**
	S4-PP11: M. BENČINA; “Bio-compatibility of stainless steel treated with advanced surface modification techniques**”.**
	S4-PP12: M.C. CIOANGHER; **“**Overcoming obstacles and finding solutions for integrating Barium Titanate–Hydroxyapatite ceramics with uncompromised piezoelectric and biological characteristics**”.**
	S4-PP13: K. DAMMAK; **“**Monovalent silver complexes based on phosphine ligands designed to promote synergistic antitumor effects**”.**
	S4-PP14: G.E. STAN; **“**Bone graft substitutes fabricated by robocasting from bioactive and piezoelectric ceramics: Pilot studies at the National Institute of Materials Physics**”.**
	S4-PP15: S. LAAFAR; **“**Temperature annealing effect on ZTO-TFT transistors performances**”.**
	S4-PP16: S. AVRAMESCU; **“**Investigating the influence of titanium and rhenium oxidation states on the catalytic properties of Ti–Re–Ox-doped materials in carbohydrate conversion to Levulinic Acid**”.**
	S4-PP17: D. OPREA; **“**Exploring antioxidant capacities and cellular effects of spring green’s polyphenolic extracts**”.**
	S4-PP18: A. ALDEA; **“**Electrospun polymeric fibers doped with natural anthocyanins for monitoring pH changes**”.**
	S4-PP19: A.M. IGNAT; **“**Study on the influence of reaction compounds on the size distribution of gold nanoparticles (AuNp)**”.**
	S4-PP20: A.E. BEJAN & **M.D. DAMACEANU**; **“**Polyimines designed for trifluoroacetic acid detection: promising materials for waveguide interferometer sensors**”.**
	S4-PP21: M.C. BUNEA; **“**Development of an electrochemical biosensor for the evaluation of enzymatic activity of methionine sulfoxide reductase A**”.**
	S4-PP22: A. BONCIU; **“**PLD-based pyramidal-shaped ceria biointerfaces**”.**
	S4-PP23: F. IACOB; **“**Gas sensing studies using polyaniline-coated chemiresistive sensors subjected to electron beam irradiation**”.**
	S4-PP24: D.D. HEREA; **“***In vitro* enhancement of antitumor drug efficacy by magnetic field-assisted rotation of gold-coated magnetic

	nanoparticles**”.**
	S4-PP25: A.I. RADU; **“**Study of ternary organic photovoltaic cells based on P3HT:PAni:Phen blend using the WO_3 mesoporous thin film as holes transport layer**”.**
	S4-PP26: C. STAVILA; **“**Silver-coated magnetite for tumor cells treatment**”.**
	S4-PP27: S. BRAJNICOV; **“**Tuning the wettability of poly(vinyl formal) polymer films via matrix assisted pulsed laser evaporation (MAPLE)**”.**
	S4-PP28: M. BRAȘOVEANU & **M.R. NEMȚANU**; **“**Enhancing starch functionality through non-thermal plasma for innovative natural-inspired materials**”.**
	S4-PP29: S. BRAJNICOV; **“**Fabrication and characterization of improved Poly(E-Caprolactone) (PCL) films for applications in biliary stents**”.**
	S4-PP30: N. LUPU; **“**Anionic dye pollutant adsorption from wastewaters by layered double hydroxide calcined material**”.**
	S4-PP31: M.E. MIHAILOV & **P. POPOV**; **“**Enhancing Romanian naval resilience to climate change: Advanced functional materials for Green Defense strategies**”.**
	S4-PP32: I. LUNGU; **“**Spectacular dispersibility of oxide nanoparticles synthesized by laser pyrolysis with isopropanol vapors as sensitizer**”.**
	S4-PP33: M.E. ZARIF; **“**Sr-doped Hydroxyapatite/ Chitosan composite layers deposited on titanium substrates for bone tissue engineering applications**”.**
	S4-PP34: L. BUDA-PREJBEANU; **“**Spiking neuron based on dual-free layer magnetic tunnel junction**”.**
	S4-PP35: R. PATRU; **“**Synthesis and characterization of functional properties in flexible ferroelectric composites with PVDF-TrFE matrix**”.**
	S4-PP36: T. TITE; **“**Enhancing perovskite solar cells efficiency by incorporating graphene oxide in the electron transport layer using electrochemical methods**”.**

Day 3, Wednesday, 17th of July 2024

Lobby of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
08:00 09:00	**Registration**						
Grand Ball Room AB – **PLENARY LECTURES (PL) SESSION** Chair: **Lucian PINTILIE**							
09:00 09:45	**PL7: Thomas SCHROEDER – "IKZ for EU: Latest R & D trends on synthesis & applications of crystalline materials"**						
09:45 10:30	**PL8: Marin ALEXE – "Symmetry breaking and novel photovoltaic effects in oxide perovskites"**						
Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
10:30 11:00	**Coffee/Tea Break**						
INVITED LECTURES (IL) & ORAL PRESENTATIONS (OP) SESSIONS							
Parallel sessions of Section 2				Craiova Hall – **S3** Chair: **Mariana Dana DAMACEANU**		Brasov Hall – **S4** Chair: **Zacharie JEHL LI-KAO**	
Grand Ball Room A – **S2** Chair: **Stefano BELLUCCI**		Grand Ball Room B – **S2** Chair: **Florencio SÁNCHEZ**					
11:00 11:30	**S2-IL5: M.R. MOLAS** "Linearly-polarized electroluminescence in van der Waals heterostructures"	11:00 11:30	**S2-IL7: M. GIRTAN** "Next materials for future opto-electronics and photonics devices"	11:00 11:30	**S3-IL5: M. NAKAJIMA** "Application of Terahertz time domain ellipsometry"	11:00 11:30	**S4-IL6: A. STROPPA** "Can we generate, tune or transfer CHIRALITY?"
11:30 12:00	**S2-IL6: I.L. PREJBEANU** "All-optical switching in magnetic memories"	11:30 12:00	**S2-IL8: V. DEMANGE** "Oxide nanosheets as seed layers for growth of complex oxides"	11:30 12:00	**S3-IL6: B. KARDYNAL** "Ultra-low energy ion implantation into two-dimensional materials"	11:30 12:00	**S4-IL7: N. AVARVARI** "Chirality Induced Spin Selectivity (CISS) effect with helicene and tetrathiafulvalene derivatives"
12:00 12:20	**S2-OP7: C.M. TEODORESCU**	12:00 12:20	**S2-OP10: R. MANU** "Thin films characterized	12:00 12:20	**S3-OP11: D. ION-EBRASU**	12:00 12:20	**S4-OP10: F. NEATU** "Acid modified MXene

	“Microscopic models of ferroelectricity in thin films and predictions of mean field theories based on them”		by the precession of the electron beam”		“PEM electrochemical hydrogen compressor evaluation”		for PET depolymerization”
12:20 12:40	**S2-OP8: J.A. HOCHHAUS** “Investigating the chemical and structural evolution of sub-monolayer Sn on Au(111)”	12:20 12:40	**S2-OP11: M. NISTOR** “New insight into the angular distribution of multi-elemental oxide thin films grown by pulsed electron beam deposition”	12:20 12:40	**S3-OP12: A.C. JOITA** “EPR investigation of the blue quartz from the Albesti - Romania granite”	12:20 12:40	**S4-OP11: I.A. BARAGAU** “Continuous hydrothermal flow synthesis of biomass-related carbon quantum dots (CQDs) as nanosensors for carcinogenic ions detection”
12:40 13:00	**S2-OP9: L. SIRGHI** “Chemical vapor deposition of octadecyltrichlorosilane monolayer films on plasma-activated silicon substrate”	12:40 13:00	**S2-OP12: F. ANDREI** “Tailoring perovskite-based thin films to boost photoelectrochemical water splitting efficiency”	12:40 13:00	**S3-OP13: C. BAROȘ** “Enabling progress in advanced materials research: Verder Scientific’s innovative solutions”	12:40 13:00	**S4-OP12: S. NEATU** “Photocatalytic water splitting using 1D-nanofilaments TiO_2-based lepidocrocite”
Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
13:00 14:30	**Lunch**						
Grand Ball Room A – S1 Chair: **Silviu POLOSAN**		Grand Ball Room B – S2 Chair: **Ioan-Lucian PREJBEANU**				Brasov Hall – S4 Chair: **Narcis AVARVARI**	
14:30 14:50	**S1-OP13: A. POPESCU & D. VIZMAN** “Numerical simulations of unsteady thermal and oxygen transport in a	14:30 14:50	**S2-OP13: K. NOUNEH** “Hierarchical nanostructure for energy and sensing application”			14:30 14:50	**S4-OP13: V.C. DICULESCU** “Portable biosensing devices for healthcare”

	Czochralski process for solar silicon growth”						
14:50 15:10	**S1-OP14: V.C. CIOMAGA HATNEAN** “Progress in the growth of crystals for optical and thermal barrier coating applications”	14:50 15:10	**S2-OP14: A. VELEA** “Advanced synthesis techniques of 2D materials for enhanced functional properties”			14:50 15:10	**S4-OP14: T.A. BURINARU** “Electrochemical impedance spectroscopy based biosensors for bleomycin detection”
15:10 15:30	**S1-OP15: L. ROMAGNOLI** “Study of thermal decomposition of formamidinium tin triiodide perovskite by means of Knudsen effusion mass spectrometry”	15:10 15:30	**S2-OP15: R. ELOTMANI** “Preparation of Cu_2SnS_3 (CTS) thin films through sulfurization of electrodeposited Cu-Sn stacked precursor layers”			15:10 15:30	**S4-OP15: A.I. BUNEA** “Micro 3D and 4D printing of pH-sensing multimaterial microrobots”
15:30 15:50	**S1-OP16: C.M. TEODORESCU** “Re-entrant ferromagnetism occurring from a simple band model as a possible origin of the geomagnetic field”	15:30 15:50	**S2-OP16: C. ENACHE** “The morphostructural and optical characteristics of SnO_2 films deposited by picosecond laser ablation”			15:30 15:50	**S4-OP16: A. ENACHE** “Advanced functional materials as trigger for fibroblasts differentiation and wound healing stimulation”
15:50 16:10	**S1-OP17: L.M. IONESCU** “On gravity and gravitational anisotropic meta-materials”	15:50 16:10	**S2-OP17: O. PANA** “Emerging properties in ferromagnetic semiconductors through interfacial charge-spin transfer in nanocomposites with			15:50 16:10	**S4-OP17: A. LŐRINCZI** “Saturation and stability tests of chalcogenide-porphyrin nanocomposite for methane sensing at environmental temperature”

			half–metals”				
16:10 16:25	**S1-OP18: W. SCHWINGER** “New workflow-based methods for material research”	16:10 16:30	**S2-OP18: H. ARDELEANU** “Study on the synthesis of gold/silver stabilized magnetite nanoparticles”			16:10 16:30	**S4-OP18: D. BOTTA** “Fabrication of a portable electrochemical cell based on flexible porous materials”
16:25 16:30	**Closing S1**						
16:30	**Coffee/Tea Break**						
16:45	**Free time to visit our Capital City ☺**						
Grand Ball Room C – D							
19:30 22:00	**Gala Dinner & Awards Ceremony**						

Day 4, Thursday, 18th of July 2024

<table>
<tr><td colspan="8">Grand Ball Room AB – PLENARY LECTURES (PL) SESSION
Chair: Lucian PINTILIE</td></tr>
<tr><td>09:00
09:45</td><td colspan="7">PL9: Adrian M. IONESCU – “Emerging nanoelectronics and artificial intelligence: Convergence, challenges and opportunities”</td></tr>
<tr><td>09:45
10:30</td><td colspan="7">PL10: Nicolae BARSAN – “Gas sensing with semiconducting metal oxides: The interplay between chemistry, physics and engineering”</td></tr>
<tr><td colspan="8">Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL</td></tr>
<tr><td>10:30
11:00</td><td colspan="7">Coffee/Tea Break</td></tr>
<tr><td colspan="8">INVITED LECTURES (IL) & ORAL PRESENTATIONS (OP) SESSIONS</td></tr>
<tr><td colspan="4"><i>Parallel sessions of Section 2</i></td><td colspan="2" rowspan="2">Craiova Hall – S3
Chair: Makoto NAKAJIMA</td><td colspan="2" rowspan="2">Brasov Hall – S4
Chair: Marin ALEXE</td></tr>
<tr><td colspan="2">Grand Ball Room A – S2
Chair: Mihaela GIRTAN</td><td colspan="2">Grand Ball Room B – S2
Chair: Cristian TEODORESCU</td></tr>
<tr><td>11:00
11:30</td><td>S2-IL9: S. BELLUCCI
“Environmental remediation through advanced carbon nanomaterials”</td><td>11:00
11:30</td><td>S2-IL11: E. KOUDOUMAS
“Novel nanostructured nanocomposites with tunable conductivity for electromagnetic shielding and potential uses in electronics and optoelectronics applications”</td><td>11:00
11:30</td><td>S3-IL7: M.D. DAMACEANU
“Current state-of-the-art characterization techniques for probing polymers as electrode materials of energy storage smart windows: A case study”</td><td>11:00
11:30</td><td>S4-IL8: A. NEMNES
“Capacitive and inductive effects in perovskite solar cells”</td></tr>
<tr><td>11:30
12:00</td><td>S2-IL10: R.W. CRISP
“Synthetic strategies, optoelectronic and physical properties of 2D nanocrystalline ABX3 chalcogenide perovskites”</td><td>11:30
12:00</td><td>S2-IL12: M.P. SUCHEA
“Complex 3D nanostructured surfaces in WO_3 thin films made by spray deposition”</td><td>11:30
12:00</td><td>S3-IL8: P. OLOWEK
“Structural characterization of nano-scaled materials using X-ray scattering techniques”</td><td>11:30
12:00</td><td>S4-IL9: A. SERGHEI
“Universal correlation between the electromagnetic interference shielding effectiveness of composite materials and</td></tr>
</table>

							their electrical properties”
12:00 12:20	**S2-OP19: I. ANTOHE** “A portable and accurate fiber optic plasmonic sensor for environmental water pollutants monitoring”	12:00 12:20	**S2-OP22: L.M. PIORAS-TIMBOLMAS** “Single qubit control in the presence of other qubits”	12:00 12:20	**S3-OP14: C.G. MIHALCEA** “Correlations between the synthesis route, morphology, structure & electrical properties of SnO_2-Gd_2O_3 nanocomposites for applications in gas sensing”	12:00 12:20	**S4-OP19: T. POTLOG** “Designing photosensitizers based on some derivatives of Zinc Phtalocyanine”
12:20 12:40	**S2-OP20: A.M. POPA** “Conductive polymers as chemiresistive ammonia gas sensing materials”	12:20 12:40	**S2-OP23: L. BUIMAGA-IARINCA** “Computational tools in material science”	12:20 12:40	**S3-OP15: M.Y. ZAKI** “Fine-tuning of S/(S+Se) ratio in magnetron-sputtered CZTSSe thin films for improved characteristics”	12:20 12:40	**S4-OP20: M.E. GHICA** “Strategies to improve the mechanical and thermal features of silica aerogels for thermal insulation applications”
12:40 13:00	**S2-OP21: T.O. CHECHE** “Atomistic approach to the strain field in finite-sized heterostructures”	12:40 13:00	**S2-OP24: L.M. PIORAS-TIMBOLMAS & L.P. ZARBO** “Fine-tuning fluxonium qubit devices for enhanced performance”	12:40 13:00	**S3-OP16: A.C. GALCA** “Facts and artifacts in optical and structural characterization of emerging materials for renewable and sustainable energy”	12:40 13:00	**S4-OP21: C.E. SIMION** “Simultaneous investigations of catalytic conversion and electrical resistance”
13:00 13:10	**Closing S2**		**Closing S2**		**Closing S3**		**Closing S4**
Foyer of J.W. MARRIOTT BUCHAREST GRAND HOTEL							
13:10 14:45	**Lunch**						

PLENARY LECTURES

(PL)

PLENARY LECTURE

PL1

The quantum revolution in metrology

Klaus VON KLITZING

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Basic research on the most important device in microelectronic, the silicon field effect transistor, led to the discovery of the quantum Hall effect and the Nobel Prize in Physics in 1985. This discovery triggered a revolution in metrology, leading to the worldwide introduction of an International System of Units based on constants of nature. For example, starting on May 20, 2019, all countries agreed to define the unit of mass, the kilogram, on the basis of a fixed value for the Planck constant h. In the same way, the unit of electrical current, the Ampere, was redefined based on a fixed value for the elementary charge e. The talk will present new insights into how the quantum Hall effect has entered this field and how the topics 2D systems and Nanostructures of the ROCAM conference contributed to this revolution.

NOTES

PLENARY LECTURE

PL2

Applications of ultra-short laser pulses in materials science

Gérard Albert MOUROU [1]

presented by Dr. **Gabriel P. BLEOTU** [2] on behalf of Prof. G.A. MOUROU[1]

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Since the first demonstration of Chirped Pulse Amplification (CPA), numerous applications, including induced nano-structuring, laser ablation, thin film deposition, ultrafast dynamics, particle acceleration, and materials characterization, have intensively utilized ultra-short laser pulses. To address the need for higher laser intensities, the nonlinear properties of transparent materials enable the post-compression of ultra-short pulses, paving the way for "extreme" light.

The generation of ultra-short and ultra-intense laser pulses and their applications in materials characterization, spectral broadening, measurements of nonlinear refractive index, and determination of laser-induced damage thresholds is discussed.

NOTES

PLENARY LECTURE

PL3

Materials for eco-design strategies for an innovative industry

Rodrigo MARTINS, Suman NANDY, Pedro BARQUINHA, Luís PEREIRA, Tomás PINHEIRO, Henrique ALMEIDA, Rui IGREJA, Emanuel CARLOS, Elvira FORTUNATO

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With the growing smartness in electronic manufacturing worldwide, printed electronics technologies draw tremendous attention because of their ability to overcome the limitation of traditional high-cost manufacturing approach which is mostly based on rigid silicon substrate. In these issues, printing technology can be used to fabricate devices on various kind of flexible substrate such as paper, textile, bendable polymers even on human skin. On the other side, printed electronics has a great potential to offer biodegradable and recyclable solutions, by choosing low-cost substrate for printing devices, that may be recycled and/or naturally degraded in nature. This is a way forward to minimize the electronic waste (e-waste) caused by the ever-increasing number of disposable electronic devices. Relevantly, "printing electronics on paper" technology is rapidly developing in both research and electronic industry fields during the last decade [1]. Generally, printing processes involve a sequence of tasks, starting with the selection of functional materials along with the envisioned functionality, moving to the formulation of inks, and then the selection of a suitable substrate. Printing technique depending on the ink's properties and intended features for the printed film. There are several printing technologies, that are being used in research and industrial sectors from lab-scale to large-scale application, such as screen printing, flexographic (or flexo-) printing, gravure printing, gravure-offset printing, and roll-to-roll (R2R) printing. A long list of functional materials, from conductive polymers, ionic liquids, and carbon nanostructures to metallic nanoparticles, and metal oxide nanostructures with conductive, semiconducting, or dielectric properties, can be used to formulate these inks [2-4]. The development of stable, cost-effective, non-toxic, and eco-friendly printable inks with desired printability is crucial to deposit and pattern these materials onto a substrate to enable the production of a new class of devices for electronics and energy purposes that are extremely lightweight, affordable, readily customizable, thin, flexible, and recyclable.

References:

[1]. S. Nandy, et al., Adv. Mater. Technol. 6 (2021) 2000994.
[2]. G. Hu, et al., Chem. Soc. Rev. 47 (2018) 3265.
[3] W. Wu, Nanoscale 9 (2017) 7342.
[4] L.W.T. Ng, G. Hu, R.C.T. Howe, X. Zhu, Z. Yang, C.G. Jones, T. Hasan, Printing of Graphene and Related 2D Materials, Springer International Publishing, 2019.

NOTES

PLENARY LECTURE

PL4

From forest to electronic and biomedical applications

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According to the United Nations University's Global e-waste monitor, a record of 62 Mt of electronic waste was generated worldwide in 2022, which represents a record in human history, up 21% in only five years. The report also predicts that global e-waste will reach 82 Mt by 2030 [1]. This makes e-waste the world's fastest-growing domestic waste stream, powered mainly by higher consumption rates of electric and electronic equipment, short lifecycles, and few options for repair. Sometimes it is mentioned that "e-waste is a toxic waste stream where valuable finite resources are lost".

The global consumption of electronics is forecast to double by 2050. In this context, printed electronics and 3D printing are an interesting alternative to conventional manufacturing methods and materials, reducing the weight of electronic components and offering more energy-efficient and sustainable solutions.

Therefore, electronics, including flexible printed circuits are facing a critical challenge: How to balance, decreasing supplies with growing volumes of e-waste? In part: by using new sustainable approaches, either in terms of materials and technological processes!

Here we propose the use of a new manufacturing technology supporting flexible and organic/inorganics electronics by exploring single laser processes for direct generation of conductive structures on biodegradable substrates. By means of different kind of laser sources, conductive carbon nanostructures can be generated on carbon-based precursor materials and substrates via a thermo-photo pyrolysis: the so-called Laser Induced Graphene (LIG). One of the main advantages of the LIG process is that the precursor materials and the substrates themselves can be bioderived and biodegradable, thus allowing new opportunities for sustainable electronics, avoiding the need to use scarce and difficult-to-recycle metal materials and be reused, in addition to costly and time-consuming processes.

In this presentation we will demonstrate the use of the LIG process to a set of devices ranging from electronic to biomedical applications.

References:

[1] https://ewastemonitor.info/the-global-e-waste-monitor-2024/

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PLENARY LECTURE

PL5

Exploring the nano-world with electrons

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In this talk, I will describe how transmission electron microscopy can be used to obtain quantitative information about not only local variations in microstructure and composition in materials, but also about functional properties and switching processes in nanoscale materials and devices. I will focus on the use of phase contrast techniques in the transmission electron microscope, such as electron holography and electron ptychography, in combination with model-based and model-independent data analysis, for the measurement of local variations in magnetic field and electrostatic potential within and outside materials with nm to atomic spatial resolution.

I will illustrate how such measurements can be made both in projection and in three dimensions, as well as in the presence of external stimuli such as applied voltage, magnetic field, reduced or elevated temperature, reactive gas and light. I will also highlight key experimental issues that need to be considered, including the influence of sample preparation, dynamical diffraction and electron-beam-induced specimen charging.

The examples that I will present will be taken from studies of individual electrically-biased phase change memory cells, arrangements of closely spaced magnetic crystals and nanoscale devices that contain geometrically-confined magnetic skyrmions, sub-100-nm vortex-like spin textures with particle-like properties that are of interest for future energy-efficient memory technologies. If time permits, I will also present examples taken from studies of electron-light-matter interactions.

This work takes advantage of the recent development of a model-based iterative reconstruction approach, which can be used to retrieve projected or three-dimensional charge density or magnetization distributions from electrostatic or magnetic contributions to recorded electron optical phase images. The approach is based on the optimized implementation of a forward model, which maps trial charge density or magnetization distributions onto experimental images. The forward model utilizes sparse matrix multiplications for efficient projections and Fourier-transform-based convolutions with pre-calculated convolution kernels based on analytical solutions for simple geometrical objects. The ill-posed problem is tackled by using least squares minimization and regularization techniques to find best-fitting solutions for reconstructed charge density or magnetization distributions.

I will conclude the talk with a personal perspective on possible future developments in instrumentation and techniques in transmission electron microscopy that may allow such measurements to be made with greater reliability, sensitivity, precision and accuracy. I will also briefly mention recent progress towards creating a sustainable distributed research infrastructure for electron microscopy in Europe.

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PLENARY LECTURE

PL6

Sustainable processes: Producing better and more with less

Paolo FORNASIERO

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Heterogeneous catalysis using readily available, well-defined, single atom or metal-free catalysts is of great interest in view of the increasing pressure on industry to move towards sustainable schemes of chemical production. In the energy sector, innovative materials have been shown to be able to efficiently convert biomass to diesel [1], liquid hydrogen carriers [2], hydrogen [3-4] also coupled with organic synthesis [5]. With the focus on sustainability in photocatalyst design, graphitic carbon nitride (g-CN) is becoming a very versatile semiconductor nanomaterial, well known for many applications. We have recently highlighted the key role that g-CN could play in the realm of photocatalytic organic synthesis, [6] and showed that tailoring the structure of g-CN by means of minimally invasive post-synthetic protocols could be the solution to tackle challenging coupling reactions with great efficiency. [7-9] Photothermal catalysts, including TiN [10], have received increasing attention even though correct temperature measurements remain difficult under those conditions [11]. All these emerging catalysts are expected to go beyond fundamental research, and will propel industrial interests toward the establishment of green organic synthesis, renewable energy conversion, pollution prevention and control [12], which represent the real challenges of modern society and the focus of the present talk.

References:

[1] N. Luo, et al., Nature Energy, 4 (2019) 575.
[2] P. Ren, et al., Joule, 7 (2023) 333.
[3] K.C. Christoforidis, et al., Nano Energy 50 (2018) 468-478.
[4] S.M. Hossein Hejazi, et al., Chem. Catal. 2 (2022) 1177.
[5] T. Montini, et al., Inorganica Chimica Acta, 520 (2021) 120289.
[6] C. Rosso, et al., ACS Nano, 15 (2021) 3621-3630.
[7] G. Filippini, et al., Sci. Adv. 46 (2020) eabc9923.
[8] A. Actis, et al., Angew. Chem. 61 (2022) e202210640
[9] E. Raciti, et al., Chem. Sci. 13 (2022) 9927.
[10] P. Fornasiero, et al., Nano Lett., 20 (2020) 3663.
[11] L. Mascaretti, et al., Joule 6 (2022 1727.
[12] M. Luna, et al., Constr. Build. Mater. 338 (2022) 127349.

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PLENARY LECTURE

PL7

IKZ for EU: Latest R & D trends on synthesis & applications of crystalline materials

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Leibniz-Institut für Kristallzüchtung (IKZ) in Berlin wishes to act as EU flagship for state-of-the-art activities in R & D on crystalline materials, supporting the EU communities by science & technology but also service & transfer. Our R & D strategy ranges from basic over applied up to pre-industrial research for electronics & photonics, including the education of young people in science & technology. In the field of electronics, I will report on our R & D on FZ-Si and ultra-wide band gap AlN and Ga_2O_3 materials for power and UV technologies; in the field of photonics, my talk will cover latest results on laser crystals, optical isolators and laser cooling.

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PLENARY LECTURE

PL8

Symmetry breaking and novel photovoltaic effects in oxide perovskites

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Symmetry is a fundamental aspect of the laws of nature and plays a crucial role in determining material properties. Breaking inversion symmetry can lead to various effects such as dielectric polarization, pyroelectricity, ferroelectricity, piezoelectricity, bulk photovoltaic effect, electro-optic effect, and second harmonic generation. Material symmetry is chiefly determined by its pristine crystallographic structure, but external stimuli can also lower symmetry or even break the inversion symmetry.

I will focus on the effects of breaking inversion symmetry in native centrosymmetric materials. I will demonstrate how built-in electrical fields within ubiquitous Schottky contacts can break the inversion symmetry at the interface, leading to piezoelectricity and pyroelectricity, and the potential for generating the "auxetic piezoelectric effect". [1,2]

I will also explore how strain gradients not only induce electric polarization but can also transform any semiconductor into a photovoltaic or photogalvanic generator through the flexo-photovoltaic effect. [3] Additionally, I will address the nonlinear transport of photoexcited carriers in $SrTiO_3$, resulting in a voltage-controlled negative resistance, resulting from an intervalley transfer of photo-induced electrons. This negative resistance can cause the photocurrent to become unstable and spontaneously produce low-frequency Gunn-like oscillations. [4] These effects, in combination with the quenching of photoluminescence by the electric field, reveal a complex band structure that warrants further in-depth investigation.

References:

[1] M.-M. Yang, Z.D. Luo, Z. Mi, J. Zhao, S. Pei E, M. Alexe, Nature 584 (2020) 377.
[2] M.-M. Yang, T.Y. Zhu, A.B. Renz, H.M. Sun, S. Liu, P.M. Gammon, M. Alexe, Nature Materials 23 (2024) 95.
[3] M.-M. Yang, K.D. Jim, M. Alexe, Science 360 (2018) 904.
[4] M. Soleimany, M. Alexe, Advanced Science 10 (2023) 2306420.

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PLENARY LECTURE

PL9

Emerging nanoelectronics and artificial intelligence: Convergence, challenges and opportunities

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The anticipated deployment of tens of billions of Edge Artificial Intelligence (Edge AI) Internet-of-Things (IoT) nodes using traditional chip technologies faces significant sustainability challenges related to energy efficiency, electronic waste, and data proliferation. Silicon nanometer CMOS technology currently dominates information processing from Extreme Edge to Cloud but is constrained by low energy efficiency, despite its widespread success across various sectors of the economy and society. The projected proliferation of IoT nodes and data volume exacerbates these challenges, hindering energy-efficient IoT deployment. Biological computing in mammalian brains, operating on spike-based information processing, is up to 10^5 times more energy efficient than CMOS technology. Biological spikes operate at much lower voltage levels compared to CMOS integrated circuits, ensuring low power consumption and effective information processing amidst noise. Classical computing architectures suffer from the von Neumann bottleneck, where data transfer between processor and memory incurs high energy costs. Neuromorphic computing, inspired by the brain`s architecture, aims to overcome this bottleneck, enhancing energy efficiency and system speed. Neuromorphic networks, including spiking neural networks (SNNs) and deep neural networks (DNNs), offer promising avenues for efficient communication and computation. SNNs, mimicking the brain`s operation with spikes in the time domain, exhibit superior energy efficiency compared to DNNs. However, DNNs have proven successful in various applications like speech and image recognition. Edge applications necessitate tiny SNN hardware for specialized tasks, operating with minimal power consumption.

To address these challenges, this talk will present our vision that involves leveraging 3D integration on silicon CMOS of emerging 2D materials and functional oxides for memristive devices, to construct bioinspired energy efficient computational blocks, like neurons and synapses, as well as sensitive spiking neurons with features beyond human senses, for future Edge AI hardware.

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PLENARY LECTURE

PL10

Gas sensing with semiconducting metal oxides: The interplay between chemistry, physics and engineering

Nicolae BARSAN

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After demonstrating their usefulness in significantly reducing the number of natural-gas-leakages related accidents, the understanding of the sensing properties of Semiconducting Metal Oxides (SMOX), and the development of better gas sensors based on them, gained a well-deserved prominence. In the last 60 years the progress was first based on the empirical improvement of the sensing materials, followed by technological improvements brought about by the combination of MEMS and thick film technologies, and by the application of chemometrics to gas sensor arrays. A SMOX based gas sensors consists of a polycrystalline, porous SMOX layer, deposited over a substrate provided with two Pt electrodes, in contact with the layer, and a heater. Typical SMOX are SnO_2, In_2O_3, WO_3 loaded with catalytic additives such as Pt, Pd and Au.

It is now well-understood that gas sensing with SMOX devices is determined by two functions: the reception and the transduction one. The former comprises the surface reactions and the accompanying charge transfer processes, which are determining the surface charge and the associated build-up of the surface space charge layers in the semiconductor. The latter determines the way in which the changes related to the reception are transformed into an electrical signal, the sensor response. This type of knowledge is the result of more recent, complex investigations, performed in the same conditions in which the sensors are operated – in Operando – combined with DFT modeling and the modeling of the conduction processes taking place in the sensing layers.

The contribution will present the way in which the understanding of the impact of both reception and transduction functions, in combination with new technological approaches, enables the development of gas sensors that are able to solve challenging applications and by that contribute to our safety and well-being.

References:

[1] N. Barsan and K. Schierbaum, Metal Oxides Series, Elsevier (2019), ISBN: 978-0-12-811224-3.
[2] N. Barsan, et al., Sens. Actuat. B 121 (2007) 18–35.
[3] A. Staerz, et al., Sens. Actuat. B 358 (2022) 131–531.

NOTES

INVITED LECTURES

(IL)

INVITED LECTURE

S1-IL1

Ag-BaTiO$_3$ CERMETs with tunable meta-composites properties

Alexandru LUKACS[1], Radu Stefan STIRBU[1], Cristina CIOMAGA[2], Liliana MITOSERIU[1], Donatella GIURANNO[3]

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The addition of metal components into dielectric matrices is a tool for increasing the effective permittivity. Recently, other interesting electromagnetic properties have been reported in such composites, which make them attractive for microwave absorption, electromagnetic shielding, filters, capacitors, etc. [1].

Ag-BaTiO$_3$ dense composites have been investigated, in searching for optimum compositions and microstructural phase arrangements providing either: (i) giant permittivity below the percolation composition, or (ii) metacomposite properties (i.e., near zero or negative permittivity), above the percolation limit. The Ag-BaTiO$_3$ composite powders have been prepared either by simple mixing of BaTiO$_3$ and Ag micropowders or by direct precipitation of Ag nanoparticles from AgNO$_3$ directly onto BaTiO$_3$ grains, in order to produce different types of dense microstructures after sintering. The idea was to exploit the interplay between the ceramic densification and silver melting/infiltration/recrystallisation in order to generate specific microstructures. For this aim, the green ceramics have been sintered at temperatures in the range of the silver melting point (900°C – 1300°C/2h) in open atmosphere. The resulting ceramics have grain sizes in the range of 350 nm – 3 μm and bi-modal distribution of silver filler, with both fine Ag inclusions and large agglomerates embedded into the ceramic matrix. The frequency and temperature dependence of the dielectric, conductive and electromagnetic properties have been investigated and discussed as a function of Ag filler addition and resulted microstructures. Modeling by 3D finite element calculations (FEM) demonstrated that dielectric, ferro/piezoelectric and tunability properties can be tailored through inhomogeneous field distributions at the interfaces between metal-ferroelectric, thus subjecting some regions to higher fields and generating enhanced electrical responses. As resulted from simulations, the frequency ranges for the metacomposite properties can be tuned by composition and microstructural design.

References:
[1] G. Fan, et al., EPJ Appl. Metamat. 8 (2021) 11.
[2] V.A. Lukacs, et al., J. Alloys & Compounds 817 (2020) 153336.

NOTES

INVITED LECTURE

S1-IL2

Multifunctional (Ba,Sr)TiO_3 systems: From nanopowders to bulk ceramics

Roxana Elena PATRU[1], Catalina-Andreea STANCIU[2,3], Vasile-Adrian SURDU[2], Elena Mirabela SOARE[2,4], Adrian-Ionut NICOARA[2], Roxana Doina TRUSCA[2], Nadejda HORCHIDAN[5], Bogdan Stefan VASILE[2], Liliana MITOSERIU[5], Ioana PINTILIE[1], Lucian PINTILIE[1], Adelina-Carmen IANCULESCU[2]

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Single-phase $Ba_{1-x}Sr_xTiO_3$ (BST x=0.10-0.40) ceramics were prepared by conventional sintering at 1400 °C for 4 h from powders synthesized via the acetate variant of the sol-gel route. The intrinsic values of the pyroelectric coefficient were determined directly from the frequency dependence of the pyroelectric signal by adapting the formalism developed for thin films deposited on thick substrates to thick and non-uniformly heated ceramics with uniform composition. The intrinsic pyroelectric properties are enhanced by increasing the Sr content, while other features decrease. The results open the possibility to use large and thick BST ceramic pellets for manufacturing detectors useful for monitoring high power lasers.

Graded structures with different architectures were obtained by spark plasma sintering (SPS) from sol-gel BST powders. The composition gradient was confirmed by structural and compositional investigations using X-ray diffraction and electron microscopy combined with energy dispersive X-ray spectroscopy. The concentration gradient was either asymmetric (3 layers, starting with x=0.10 and ending with x=0.30) or symmetric (5 or 6 layers, starting and ending with x = 0.10). Dielectric constant decrease with increasing of the layers number. The symmetric graded structure with 6 layers has the best thermal stability of both, the dielectric constant and the pyroelectric coefficient. An enhancement of the pyroelectric signal for frequencies above 100 Hz is obtained in symmetric structures, effect attributed to the additive contributions of the signals originated from the layers with different Sr content.

The SPS consolidation technique was also used to produce dense, homogeneous, fine-grained $Ba_{0.8}Sr_{0.2}TiO_3$ (BST20) and $Ba_{0.6}Sr_{0.4}TiO_3$ (BST40) ceramics starting from sol-gel nanopowders, with mean particle size values of 68 and 70 nm, respectively. The purpose of this approach was to investigate the influence of the so-called size effects on the functional properties of BST ceramics. By decreasing grain size (GS) from the submicron toward the nanometre range, an increase of the phase transitions diffuseness accompanied by a decrease of both the permittivity maxima and the dielectric losses, was revealed by broadband dielectric spectroscopy. For BST20 ceramic, the Curie-Weiss temperature, as well as the Curie constant decreases when grain size is diminished, indicating an overall reduction of the ferroelectric active volume, as a grain size reduction effect. High field P-E measurements have shown that the hysteretic behavior decreases when reducing the GS. For BST40 sample, the field-dependent permittivity changes its shape from butterfly to slim, but nonlinearity is still noticed even for the nanocrystalline specimen. Nanostructuring determines the increase of the electrostatic energy storage capability and efficiency due to the reduction of hysteretic character.

NOTES

INVITED LECTURE

S1-IL3

Enhancing the mechanical properties of carbon nanotube materials through computationally guided engineering of interactions between fibers at the mesoscale level

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While molecular dynamics methods can quantify the nano-mechanical properties at the carbon nanotube (CNT) pristine, polymeric, and cross-linked interfaces, they become impractical when it comes to predicting their impact within CNT assemblies. Using the mesoscopic distinct element method (MDEM) for CNTs, we can perform coarse-grained multiscale simulation to compare the impact of polymeric and cross-linking interfaces in highly discontinuous CNT bundles and network assemblies subjected to simple tension. Viscous friction and contact shear bonds are used in MDEM to capture the polymeric and cross-linking nano-mechanics computed separately with atomistic methods. For example, interacting nanohole defects modeled with density functional theory-based tight-binding molecular dynamics, were used as model systems for radiation-treated, flattened CNTs. These covalent cross-links improve the load transfer between CNTs, while the nanoholes reduce the in-plane mechanical properties. The computed catalog of interacting nanohole defects is used to inform mesoscopic models of irradiated CNTs. MDEM simulations find that cross-linking is more effective than polymeric bonding at increasing elastic moduli and tensile strengths of the CNT bundles. These properties can be diminished by the nano-holes in the CNT wall associated with irradiation-generated cross-linking and captured here into the contacts representing CNT stretching. Simulations indicate the need to balance the benefits and drawbacks of the radiation-induced morphological changes to manufacture CNT yarns with superior tensile characteristics. The MDEM utility will be further showcased in simulations of the densification processes and fabrication of nanostructured metasurfaces of nanometer-thin CNT films obtained from aerosol chemical deposition reactors, where atomic force microscope lithography demonstrated nanoscale patterning.

NOTES

INVITED LECTURE

S2-IL1

Disentangling stress and strain effects in ferroelectric HfO_2

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Ferroelectric HfO_2 films are usually polycrystalline and contain a mixture of polar and nonpolar phases. This challenges the understanding and control of polar phase stabilization and ferroelectric properties. Several factors such as dopants, oxygen vacancies, or stress, among others, have been investigated and shown to have a crucial role on optimizing the ferroelectric response. Stress generated during deposition or annealing of thin films is a main factor determining the formed crystal phases, which has an obvious effect on the ferroelectric polarization of the films. But stress also influences the lattice strain of the polar orthorhombic phase. It is difficult to discriminate between stress and strain effects on polycrystalline ferroelectric HfO_2 films due to the coexistence of polar and non-polar polymorphs, and the direct impact of orthorhombic lattice strain on ferroelectric polarization has yet to be determined experimentally. Here, we analyze the crystalline phases and lattice strain of several series of doped HfO_2 epitaxial films. We conclude that stress has a critical influence on metastable orthorhombic phase stabilization and ferroelectric polarization. On the contrary, the lattice deformation effects are much smaller than those caused by variations in the orthorhombic phase content. The experimental results are confirmed by density functional theory calculations on HfO_2 and $Hf_{0.5}Zr_{0.5}O_2$ ferroelectric phases.

NOTES

INVITED LECTURE

S2-IL2

Hafnia-based ferroelectric field effect memristor synapses epitaxially grown on silicon

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Ferroelectric tunnel junction (FTJ) memristors first implemented by perovskite ferroelectrics [1], require low ferroelectric thickness in the range on 3-4 nm. However, ferroelectricity in $Hf_{0.5}Zr_{0.5}O_2$ (HZO) becomes metastable [2] below 10 nm due to depolarization fields and, with few exceptions, diminishes below 5 nm. To overcome the problem, a new ferroelectric field effect memristor is proposed, comprising 5 nm epitaxial HZO ferroelectric with 10 nm epitaxial $SrTiO_3$-δ (STO) semiconductor bottom electrode, all monolithically integrated on silicon (001) [3]. From XRD pole figure analysis and HRTEM it is inferred that HZO is epitaxially grown on STO due to domain matching epitaxy [4] albeit with 90, 180 and 270 deg rotated domains due to the 4-fould symmetry of the substrate. The STO is deliberately n-type doped with O vacancy donors to act as a bottom electrode. The HZO shows a polarization of 14×10^{-6} C/cm^2 and a very low coercive voltage of < 1 V. It is anticipated that the ferroelectric polarization charges deplete or accumulate the semiconductor surface thus modulating the total junction resistance through a quasi-continuous spectrum of resistance states producing an analog non-volatile memory. The polarization also induces oxygen vacancy movements in the STO and redox reactions [5] at the interface which contribute to the resistance modulation in an additive way amplifying the effect.

Due to the beneficial combination of electronic and ionic effects, the memristor shows several forms of synaptic plasticity [3]. Nearly ideal symmetric and linear potentiation and depression were obtained with time correlated identical pulses. Pair pulse facilitation and spike timing dependent plasticity is obtained in several time scales from more than 1 ms down to 100 ns and for very low programming voltage from 2 V down to 0.4 V, in compatibility with voltage scaling of CMOS. The devices show no retention loss for more than 4×10^4 sec pertaining to the low resistance state and several inter-mediate states. Endurance of ON and OFF states with 3 MV/cm cycling fields is 106 cycles, while the endurance of intermediate states with lower cycling fields of 1.0-1.8 MV/cm is better well exceeding 10^6 cycles. As a voltage driven memristor, the device is estimated to consume less than 10 fJ per programming event which is comparable to biological synapses. The performance of our ferroelectric memristors makes them a good candidate for analog in-memory computing in dense and large cross bar artificial intelligence accelerator arrays where power consumption and cross talk due to sneak paths are big concerns.

References:
[1] A. Chanthbouala, et al., Nat. Mater. 11 (2012) 860; D.J. Kim, et al., Nano Lett. 12 (2012) 5697.
[2] N. Siannas, et al., Comm. Phys. 5 (2022) 178. [3] N. Siannas, et al., Adv. Funct. Mater. 34 (2024) 2311767.
[4] S. Estandia, et al., Cryst. Growth Des. 20 (2020) 3801.
[5] R. Dittmann, S. Menzel, R. Waser, Adv. Phys. 70 (2021) 155–349.

NOTES

INVITED LECTURE

S2-IL3

Unveiling nonlinear optical and electrical responses in molybdenum disulfide: A journey through 2D materials and beyond

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A pronounced second harmonic generation (SHG) response is observed from the single-layer edges of the nanoribbons, attributed to symmetry breaking. This contrasts with the multilayer structure, which is less responsive to the second-order nonlinear process. Raman spectra analysis reveals distinct spectral features attributed to monolayer edges and the multilayer core, resulting in a notable split of the Raman spectra of the MoS_2 nanostructures. Tip-enhanced photoluminescence imaging shows a blue-shifted exciton emission from nanoribbon edges compared to isolated monolayers, attributed to local strain and disorder [2]. Moreover, the MoS_2 nanoribbons exhibit strong polarization-dependent Raman, optical, and electrical response. Polarization-dependent SHG analysis confirms that the multilayer core of the nanoribbons exhibits predominantly a 2H stacking orientation. On the contrary, we did not observe any polarization dependency for the 2D triangular MoS_2 crystals [3]. The growth of such anisotropic MoS2 nanoribbons opens a wide range of applications in polarization-sensitive optoelectronic devices. Finally, we will present an ultrasensitive photodetector constructed from a single MoS_2 nanoribbon. It boasts a responsivity of 8.72×10^2 A/W (gate voltage +80 V) under 532 nm laser illumination, among the highest reported for single-nanoribbon photodetectors. These findings offer insights into the design of MoS_2 semiconductors with adaptable geometries for efficient optoelectronic devices.

References:

[1] D.I. Miakota, G. Ghimire, R. Ulaganathan, M. Rodriguez, S. Canulescu, Appl. Surf. Sci. 619 (2023) 156748.
[2] G. Ghimire, R.K. Ulaganathan, A. Tempez, O. Ilchenko, R.R. Unocic, J. Heske, D.I. Miakota, C. Xiang, M. Chaigneau, T. Booth, P. Boggild, K.S. Thygesen, D.B. Geohegan, S. Canulescu, Adv. Mater. 35 (2023) 2302469.
[3] G. Ghimire, R.K. Ulaganathan, A. Tempez, O. Ilchenko, R.R. Unocic, J. Heske, D.I. Miakota, C. Xiang, M. Chaigneau, T. Booth, P. Boggild, K.S. Thygesen, D.B. Geohegan, S. Canulescu, under preparation (2024).

NOTES

INVITED LECTURE

S2-IL4

Towards developing emerging antimony and bismuth-based chalcogenide for next generation, Earth abundant photovoltaics

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The emergence of new PV applications in the society requires design of materials and devices with a different set of properties. At this scale, for a new photovoltaic (PV) technology is not sufficient to be only competitive with the Si and CdTe technologies in efficiency and reliability but one should also rely on green, environmentally friendly, and earth-abundant materials. An emerging class of highly promising PV materials currently under widespread investigation in the PV community are the inorganic antimony-and bismuth-based chalcogenide compounds. The excellent intrinsic material properties of these compounds allowed to rapidly approach 8-10% conversion efficiency, opening a new chapter in PV research, full of new possibilities but also scientific challenges. This talk will discuss the latest achievements in bismuth- and antimony- based thin film solar cell technology with the main emphasis on Sb_2Se_3, Sb_2S_3 and Bi_2S_3 compounds. I will summarize the knowns and unknowns of their defect chemistry, including highlights of unique optoelectronic characteristics that are not yet fully explained. The discussion will highlight the progress achieved in our group, toward growth of high-quality Sb_2S_3, Sb_2Se_3 and Bi_2S_3 absorber films and solar cells by rapid, high-volume, and in-line close-spaced sublimation and vapor transport deposition techniques. Special emphasis will be put on the key processing strategies to optimize absorber material properties (doping and alloying), understanding of buried interfaces and push the boundaries of understanding and performance. A thorough look at the formation chemistry and shed light on some of the synthesis and doping challenges, potential doping elements, the impact this has on carrier density and the impact on solar cell performance.

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INVITED LECTURE

S2-IL5

Linearly-polarized electroluminescence in van der Waals heterostructures

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Germanium sulfide (GeS) is an anisotropic layered material with a direct band gap around 1.78 eV [1]. GeS possesses a low-symmetry orthorhombic crystal structure analogous to that of black phosphorous. The optical response of GeS was systematically investigated using experimental techniques, such as photoluminescence, reflectance contrast, and Raman scattering [2]. Electroluminescence (EL) studies have not been reported in the literature yet. The investigation of EL anisotropy is an innovative aspect of this study.

In this work, we investigate the EL response of GeS assembled in two types of structures: with tunnel barriers and without tunnel barriers. Thin layers of hexagonal BN (hBN) act as tunnel barriers. The bias voltage was applied to the graphene flakes via metallic contacts.

The EL of the sample with tunnel barriers is apparent at 1.77 eV, which is associated with the neutral excitonic transition in GeS. It is intriguing that the structure without tunnel barriers does not have EL from the neutral exciton. However, there are observed emissions at higher energies at 2.04 eV and 2.30 eV, which coincide with higher energy transitions around the Γ point. In the sample with barriers, GeS exhibits linearly polarized EL along the armchair crystallographic direction, which is in agreement the corresponding photoluminescence response [2].

References:

[1] M. Arfoui, et. al., Nanoscale 15 (2023) 17014.
[2] N. Zawadzka, et. al., Nanomaterials 11 (2021) 3109.

NOTES

INVITED LECTURE

S2-IL6

All-optical switching in magnetic memories

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The evolution of computer memory has led to a multilevel hierarchy, balancing speed, storage density, and cost. As complementary semiconductor memory limits are approached, interest grows in nonvolatile alternatives like magnetic random access memory (MRAM). Although perpendicular spin-transfer torque is already in production, alternative technologies such as spin-orbit torque (SOT) are explored for high-speed and fast cache operation. However, SOT has drawbacks, such as a larger bit-cell area and the need for an applied magnetic field for deterministic switching. In the pursuit of faster, more efficient memory, all-optical switching (AOS) technology seeks to achieve magnetization reversal through energy-ecient ultrafast writing with single-femtosecond laser pulses. This work addresses the objective of merging helicity-independent HI-AOS with MRAM devices. The materials investigated are rare-earth transition-metal multilayer systems, with a particular focus on Tb/Co-based structures. Through a combination of experimental investigations and numerical simulations, we unraveled the intricate dynamics of HI-AOS and used them to develop functional nanometer-sized AOS magnetic tunnel junctions (AOS-MTJs). The exploration of HI-AOS in thin films of rare-earth transition metal multilayer systems lays the foundation for reliable magnetization toggle reversal, exploring the response to different pulse durations and fluences. Key new findings include the observation of concentric rings with opposite magnetic orientations and the independence of fluence on pulse duration, challenging existing paradigms. Practical applications require the fabrication and electrical characterization of MTJ devices. Optimization of tunnel magnetoresistance (TMR) values, reaching a maximum value of 74%, a significant improvement over previous demonstrations. The thesis main achievement was demonstrating field-free HI-AOS on 100 nm diameter patterned [Tb/Co] p-MTJ devices, using 50 fs laser pulses with an estimated absorbed energy of approximately 68.6 fJ per bit reversal. This work offers a comprehensive exploration of HI-AOS, from its fundamental mechanisms to practical applications in nonvolatile data storage and energy-ecient computation. The optimized TMR values and successful demonstration of AOS in nano-patterned devices are a first step toward a new memory technology. The use of both experimental and simulated methods strengthens the importance of the obtained results for further progress in this area. Our results expanded the knowledge of helicity-independent all-optical switching but has also laid the foundation for innovative applications in nano-scale technology. The ongoing integration of photonic and spintronic elements has the potential to bring about significant progress in data storage and computation.

NOTES

INVITED LECTURE

S2-IL7

Next materials for future opto-electronics and photonics devices

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The process of the transmission of an information passes today by a binary codification. This digitalization codification allowed to associate to each word an equivalent transcription in a binary code with a series of sequences of numbers of zero and one. Hence by using a presence of something "1" or an absence "0" we can "write" and transmit an information similarly to the transmission in Morse code. On this principle, today, in the place of sounds, electrons and photons are used as carrier information vectors and the data transmission is done by electrical and optical pulses. Besides, other information carrier vectors can be imagined and used such as: plasmons, spin, magnons, etc.

The new materials for electronics and photonics devices are carbon-based materials such as: polymers, graphene, $CH_3NH_3PbI_3$ and related perovskite compounds, paper etc. The advantages of these materials are that they are abundant, compatible with the deposition of thin films on flexible light substrates and large area by low-cost depositions technologies such as inkjet or roll to roll. Beside their excellent mechanical properties, polymers and 2D materials such as graphene present also very interesting electrical and optical properties for electronics and photonics devices. These technologies allowed last years to successfully develop devices for data transmission. In this paper a complete characterization from optical, morphological and electrical point of view was done for PEDOT:PSS for $CH_3NH_3PbI_3$ thin films. Th electrical photoconductivity allowed the calculation of different relaxation time and allow to give important information concerning the suitability of the use of these materials for photonics devices. Also, these time depending experiments allow to explain better the behavior of these films used in OPV and PKV solar cells and can complete the understanding of data and experimental observations concerning the solar cells behavior.

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INVITED LECTURE

S2-IL8

Oxide nanosheets as seed layers for growth of complex oxides

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Functional properties such as ferroelectric, multiferroic or transparent conducting oxide in complex oxide thin films are key components in modern devices. Their properties are related to their orientation and to their structural and microstructural qualities in relation with the crystal growth. Epitaxial films are obtained on single-crystalline oxide substrates (such as $SrTiO_3$) that present chemical compatibility and small in-plane lattice parameters mismatch with the film. However, these substrates are expensive and size-limited. On the other hand, direct growth of functional oxides on low-cost substrates with large area as silicon or glass leads to amorphous or polycrystalline films with poor properties. Therefore, introduction of a buffer layer is necessary on such substrates in order to achieve the epitaxial growth of complex oxides. Among other candidates, oxide nanosheets have been identified for several years as seed layers to induce the preferential growth of complex oxides with a high crystalline quality, on several low-cost substrates as silicon, glass, mica, polymers and metallic foils [1,2]. These nanosheets are obtained by exfoliation of layered oxides, as $KCa_2Nb_3O_{10}$, $K_{0.8}Ti_2O_4$, K_xMnO_2 [2]. They possess either 2D square, rectangular or hexagonal lattices, allowing regrowth of [001], [011] and [111] preferentially oriented perovskite oxides. The nanosheets are transferred on low-cost substrates by drop casting methods [3], which allow a high surface coverage of the substrate. As example of epitaxial growth, we will show the possibility to integrate complex oxide perovskites thin films grown by pulsed laser deposition, such as $La_{0.67}Sr_{0.33}MnO_3$ [4], $KNbO_3$ [5] and $SrVO_3$ [6] on glass, silicon and mica.

References:

[1] M. Arfoui, et. al., Nanoscale 15 (2023) 17014.
[2] N. Zawadzka, et. al., Nanomaterials 11 (2021) 3109.

NOTES

INVITED LECTURE

S2-IL9

Environmental remediation through advanced carbon nanomaterials

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In this study we demonstrate the effectiveness of modified multi-walled carbon nanotubes (MWCNTs) in adsorbing and photodegrading tartrazine, a model pollutant. Two types of nanocomposites were prepared: MWCNT-COOH/Fe_3O_4 and MWCNT-COOH/Fe_3O_4/NiO. These nanocomposites were synthesized by precipitating metal oxides in the presence of MWCNTs. The properties of the nanocomposites were thoroughly examined using various techniques including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), scanning electron microscopy (SEM), Raman spectroscopy, synchrotron-based Scanning PhotoElectron Microscopy (SPEM), and Brunauer-Emmett-Teller (BET) analysis. These analyses provided insights into the structure, composition, and morphology of the nanocomposites [1].

We determined the optimal conditions for adsorption of tartrazine onto the nanocomposites. For MWCNT-COOH/Fe_3O_4, the optimal pH was found to be 4, while for MWCNT-COOH/Fe_3O_4/NiO, it was pH 3. Other optimal conditions included a temperature of 25 °C, adsorbent dose of 1 g L−1, and specific initial concentrations of tartrazine. Additionally, contact times for adsorption were determined. We elucidated the predominant degradation process of tartrazine, both with and without simulated sunlight irradiation. Thermal lens spectrometry (TLS) and UV–Vis absorption spectrophotometry were employed to analyze the degradation process. The results indicated that photodegradation was the prevalent mechanism, surpassing adsorption, from the initial stages of the degradation process.

For the removal of Cationic Pollutants we also used Oxidized Graphene: here the focus is the effective and efficient removal of cationic pollutants from aqueous solutions using oxidized graphene. The advantages of this adsorbent material are: fast adsorption and good efficiency over a wide range of initial pollutant concentrations and pH values; green adsorbent based on the use of oxidized graphene as an eco-friendly material for wastewater decontamination. Herein, pristine reduced Graphene Oxide—prepared by an eco-friendly protocol—is used for the removal of cationic pollutants from water, i.e., methylene blue (MB) and mercury-(II) (Hg-(II)) [2-4].

Acknowledgments:

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References:

[1] Stegarescu A., et al., Nanomaterials 12 (2022) 3008.
[2] Tene T., et al., Nanomaterials 12 (2022) 309.
[3] Tene T., et al., Nanomaterials 12 (2022) 3025.
[4] Tene T., et al., Coatings 12 (2022) 1154.

NOTES

INVITED LECTURE

S2-IL10

Synthetic strategies, optoelectronic and physical properties of 2D nanocrystalline ABX3 chalcogenide perovskites

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Investigating materials to discover and utilize new properties is key for driving technological progress. Perovskite materials offer remarkable properties regarding light absorption, charge transport, and application in highly efficient solar cells. However, since the best performing type of perovskites contain lead (Pb) – a toxic heavy metal, banned for commercial use in the EU – we seek new materials that do not rely on Pb or Cd (another toxic element commonly used in solar cells). A flexible method to investigating alternative materials is through colloidal nanocrystal synthesis. Colloidal synthesis of materials provides routes to obtaining materials with tailored, controlled properties using relatively straightforward experimental apparatuses. We present first work on the fabrication of earth-abundant ternary chalcogenide Perovskite-like 2D nanocrystals of low-toxicity as well as their potential usage in PV devices. The optoelectronic properties of these materials ($BaZrS_3$, $BaTiS_3$) are characterized with absorbance, emission, Raman, and transient absorption spectroscopies as well as the physical characteristics using XRD, TEM, and EDX. We find the crystal structure for each material depends on the starting metal precursors used to prepare the colloids and that the crystal habit can be changed based on growth temperature yielding spheres, rods, or nanoplatelets. Furthermore, films are to prepare exploratory heterojunctions with ZnO as the electron transporting material. These materials show promise for photoactive devices, but further optimization is needed. However, the paths forward will be presented and discussed with focus on layer processing, device configurations, and material properties.

References:

[1] Stegarescu A., et al., Nanomaterials 12 (2022) 3008.
[2] Tene T., et al., Nanomaterials 12 (2022) 309.
[3] Tene T., et al., Nanomaterials 12 (2022) 3025.
[4] Tene T., et al., Coatings 12 (2022) 1154.

NOTES

INVITED LECTURE

S2-IL11

Novel nanostructured nanocomposites with tunable conductivity for electromagnetic shielding and potential uses in electronics and optoelectronics applications

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Electromagnetic interference (EMI) can disrupt the operation of electronic devices, equipment and systems, as well as can affect life. With the new generation of communications at 5G technology, EMI shielding becomes quite important, since, as frequency increase, so interference does. As a result, without proper shielding, our brand-new phones or other electronic equipment might not work in the right way. The present work concerns the design, synthesis, and characterization of novel rare earth elements doped metal oxide-graphene nanocomposites materials with tunable conductivity suitable for the shielding of electromagnetic radiation in the >5GHz spectral range. The ZnO:RE/Graphene (RE: Er, La, Sm) nanocomposite materials were obtained using a two stages method: electrospinning of precursor solutions followed by calcination at 600 °C (for 2 hours in N_2 medium). All materials show a granular structure formed by nanocrystallites agglomerations randomly distributed in a lace-like and flakes-like matrix. Materials nanostructuring was found to be strongly affected by the nature of the dopant. Er dopant was found to lead to "aeration" of the nanomaterial promoting the formation of the lace-like matrix that suspends nanosized granular nanoparticles, while, in the case of La doping, the respective nanoparticles were smaller and the matrix was more compact. Sm doping resulted in smaller size nanoparticulates embedded in a porous 3D lace-like foamy matrix. The materials were found to exhibit a quite interesting conductivity variation as a function of frequency, since, this was presenting a considerable increasing for higher frequencies and temperatures. Simulations were performed to explain the unusual behavior of these materials. According to the theoretical and experimental observations, it seems that ZnO:RE/Graphene (RE: Er, La, Sm) nanocomposite materials may be excellent candidates to be used as tunable bandgap semiconductors in electromagnetic shielding applications.

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INVITED LECTURE

S2-IL12

Complex 3D nanostructured surfaces in WO_3 thin films made by spray deposition

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The talk will present our recent studies regarding the evolution of a unique 3D structured surface of tungsten oxide (WO_3) thin films made by spray deposition, not yet studied in detail, consisting of a complex combination of nano-balls and walls-like features. Since the surface morphology and structure play a crucial role in most optoelectronic applications, and WO_3 is one of the most important metal oxide semiconductors in a huge variety of these applications, a detailed study of these, recently observed and reported, unique 3D complex architecture of WO_3 films is of great importance for further development of films and devices. In this context, series of WO_3 films with different thicknesses and made with different tungsten peroxide precursor concentrations were fabricated by spray pyrolysis. The samples were thoroughly characterized by field emission scanning electron microscopy (FE-SEM), X-ray diffraction and Raman spectroscopy. Results suggest that, for the employed fabrication parameters, the main differences in the structure affect mostly the surface morphology and slightly the surface texturing. These observations prove the viability of the fabrication by the spray pyrolysis of coatings with such surface morphology and open new perspectives for better sensors, electrochromic and photochromic devices, etc.

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INVITED LECTURE

S3-IL1

Carrier-resolved photo-Hall effect

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Majority and minority carrier properties represent fundamental parameters governing semiconductor device performance. Obtaining this information simultaneously under light illumination would unlock many critical parameters such as recombination lifetime, recombination coefficient, and diffusion length; while of critical importance for optoelectronic devices and solar cells, this goal has remained elusive. Studies to collect both majority/minority carrier properties for high-performance light absorbing materials have been attempted, but require a wide range of experimental techniques, which typically use different sample configurations and illumination levels thereby presenting additional complications in the analysis. Here, we demonstrate a carrier-resolved photo Hall technique that rests on a new identity relating hole-electron Hall mobility difference, Hall coefficient and conductivity. This discovery, together with advances in ac-field Hall measurement using a rotating parallel dipole line system, allows us to unlock a host of critical parameters for both majority and minority carriers. We successfully apply this technique to various light absorbers such as Si, $Cu_2ZnSn(S,Se)_4$, organometal lead halide perovskites, $(FA,MA)Pb(I,Br)_3$ and map the results against varying light intensities, demonstrating unprecedented simultaneous access to these parameters.[1] This information, buried in the photo-Hall measurement, has so far been elusive for 140 years since the original discovery of Hall effect. Beyond historical significance, the applications of simultaneous majority and minority carrier measurement are broad, including photovoltaics, optoelectronics and various electronic devices.

Reference:

[1] O. Gunawan, S.R. Pae, D.M. Bishop, Y. Virgus, J.H. Noh, N.J. Jeon, Y.S. Lee, X. Shao, T. Todorov, D.B. Mitzi, B. Shin, Nature 575 (2019) 151–155.

NOTES

INVITED LECTURE

S3-IL2

Analysis of buried interfaces for device technology by soft and hard X-ray photoemission

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Due to its accuracy and reliability in determining nm-thick overlayers on Si, XPS has been utilized as a metrology technique for many years. It has become more challenging to perform surface sensitive XPS with a soft X-ray source because the interfaces of interest are frequently hidden beneath metal electrodes or oxide layers. Higher energy X-ray probe beams have made it possible to gather photoelectron signals from further deep in the material thanks to the development of lab-based hard X-ray spectrometers (HAXPES). New options for routine application for the qualification of the procedures and components utilized in technologically significant devices are thus made available. In this talk, we will discuss the current state of the art and possible future directions for integrating hard X-ray photoelectron spectroscopy (HAXPES) and soft X-ray photoelectron spectroscopy (XPS) in the study of semiconductors and nanoelectronics. We`ll discuss the benefits of employing Hard X-ray sources on a lab-based high throughput fully automated spectrometer. This includes analysis of buried interfaces, such as electronic layers below a surface capping layer, and compositional studies in the bulk of materials and interfaces below the sampling depth of soft X-rays. Reduced surface contamination`s impact on the photoelectron signal is another benefit of deeper sampling. For precisely the same reason, a deeper sample depth of the Cr source enables one to explore past the potential depth of ion sputtering-induced damage. Another crucial benefit is eliminating the overlap between Auger and major photoemission peaks. This is particularly important for transistor devices based on GaN technology, for which quantification using XPS is impossible due to the overlap between Ga Auger peaks and N 1s photoelectron peaks. Thin films of various types are critical components of modern microelectronic products. Conducting films form the interconnect layers in all chips, and dielectric films provide electrical insulation. Angle-resolved or angle-dependent XPS and HAXPES (ADXPS/ADHAXPES) is a powerful, non-destructive method that provides a quantitative chemical composition depth profile for thin film structures with thicknesses within the XPS sampling depth - under 5 – 10 nm for an Al K alpha soft X-ray source and ~15 – 30 nm for a Cr K alpha hard X-ray source. We will describe the use of the software StrataPHI for metrological applications in devices to estimate the structure of thin-film stacks from angle-dependent and spectral XPS and HAXPES data.

NOTES

INVITED LECTURE

S3-IL3

Design, fabrication and characterization of adaptive electron-optical devices for beam shaping

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Adaptive electron-optical phase plates, devices that can shape the illumination in amplidue and phase, are revolutionizing electron microscopy. They are composed of a set of active elements, electrodes, current segments, light beams, that can be tuned and controlled externally to realize the analogue of what in light optics are known as spatial light modulators. Their implementation and operation provide us with new and powerful methods that broaden the reach of coherent electron imaging. Typically, adaptive phase plates are based on MEMS technology to facilitate their implementation in a transmission electron microscope. Even so, their fabrication is a complex task that involves sophisticated clean-room techniques, a positive interplay of materials, and electrical engineering to interface the devices inside the microscope with the outside world. These devices can be placed either before the sample, to structure the illumination in a way that synergizes with the sample features we are interested in -this is the concept of resonant imaging-, or after the sample, typically in the objective aperture or selected area planes, to analyze the electron wave function emerging from the sample in ways that are not feasible with conventional electron-optical elements (lenses, deflectors, prisms, etc.). A clear example of this is the Orbital Angular Momentum sorter, a post-sample dual phase plate system that allows us to measure the angular momentum components of an arbitrary wave function. Once fabricated, adaptive phase plate requires a validation of their intended functionality. This is accomplished by provisionally inserting them at the sample plane of the microscope as objects to study. Since the active beam-shaping elements are electric and/or magnetic fields, we need imaging methods that are sensitive to them. The family of coherent electron imaging techniques, including electron holography and interferometry, Lorentz imaging and Transport of Intensity, provide us with the necessary tools for such investigation. In this presentation we will discuss several designs of adaptive phase plates, accompanied by 3D finite element simulations illustrating the electromagnetic field they produce and the expected beam-shaping functionality. Then, we will focus on a specific adaptive phase plate intended for dynamic aberration correction and illustrate its fabrication, implementation and preliminary experimental validation.

NOTES

INVITED LECTURE

S3-IL4

X-ray diffraction for battery analysis: Modern challenges and modern solutions

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With the ever-increasing demand for new and improved battery materials, efficient characterization methods to obtain precise insights into both raw materials and fully assembled batteries are more important than ever. Since most modern battery materials are crystalline, and the crystallinity and crystal structure can have a significant influence on a material's performance, X-ray diffraction (XRD) is one of the go-to methods both for operando structural characterization of assembled batteries, and for ex situ investigation of battery raw materials or recycling products. The large variety in battery materials, and the many different shapes and sizes of commercial cells pose certain challenges for XRD instrumentation. As many active materials only show slight structural differences from one another, such as the substitution of cobalt in LCO with similarly sized nickel and manganese to obtain NMC, high quality diffraction data that allows the precise determination of lattice parameters is essential.

Additionally, high energy X-rays are required to penetrate the airtight metal housings surrounding assembled batteries. For this reason, the availability of high energy X-ray sources (e.g., molybdenum or silver), and suitable optical components and detectors, is crucial.

Finally, dedicated battery sample holders that allow precise positioning and reliable electrical connection of batteries for operando measurements round off the requirements for modern, high-quality powder X-ray diffractometers for battery analysis.

In this presentation, a variety of challenges and solutions for XRD measurements on batteries will be discussed, covering both operando measurements on fully assembled batteries and ex situ analysis of raw materials. An overview of the state-of-the art in XRD on batteries, from cell assembly to sample holders and measurement setup will also be presented.

NOTES

INVITED LECTURE

S3-IL5

Application of Terahertz time domain ellipsometry

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Terahertz time domain ellipsometry is an emerging characterization technique to study various materials` dielectric and conductivity properties. The terahertz region refers to the frequency band between the millimeter and infrared waves of the electromagnetic spectrum, and in this region many low-energy excitations are present such as free carriers, phonons, plasmons, magnon and rotational transitions. The carrier dynamics that occur at terahertz frequencies also elucidate the optical properties of materials. Hence, terahertz investigations are employed in studying next-generation materials such as wide-bandgap semiconductors and other functional materials [1–3].

In the terahertz ellipsometry the material properties are probed by irradiating polarized terahertz pulses and then measuring the change in the polarization state of the reflected waves. The ellipsometric parameters reflect the properties of the dielectric and free carrier responses, such as carrier density and mobility. We succeeded in developing the high-precision terahertz time-domain ellipsometry. We will demonstrate some experimental results in the wide-bandgap semiconductors of GaN and so on at the conference. Our terahertz ellipsometry system can evaluate the wider carrier density range up to 10^{21} cm^{-3} compared to conventional terahertz time domain spectroscopy.

References:

[1] V.C. Agulto, M. Nakajima, et al., Sci. Rep. 11 (2021) 18129.
[2] V.C. Agulto, , M. Nakajima, et al., Appl. Phys. Lett. 118 (2021) 042101.
[3] T. Iwamoto, M. Nakajima, et al., Jpn. J. Appl. Phys. 62 (2023) SF1011.

NOTES

INVITED LECTURE

S3-IL6

Ultra-low energy ion implantation into two-dimensional materials

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Ion implantation is a well-established, key technological process for doping bulk semiconductor devices. Irradiation of two-dimensional materials with the typically used ion energy in the range of tens of keV is not efficient for ion implantation as the most likely outcome of such a process is the creation of vacancies. In this talk, we will present the results of our studies aiming at optimization of ion implantation of two-dimensional semiconductors on the examples of transition metal dichalcogenides and thin layers of hexagonal boron nitride. We will show that substitutional doping in monolayer semiconductors is possible with ion energies of tens of electronvolts. We will discuss the conditions for site-selective implantation at high implantation rates. Further, we will show that the defects introduced by ion irradiation depend not only on the choice of the ions and their energy but also on the choice of the implanted material and the substrate as predicted by ab-initio calculations. In analogy to the ion implantation into bulk materials, post-implantation annealing can be used to remove defects and the annealing conditions are also subject to the nature of the defects and the choice of implanted material. Considering the influence of the substrate and the need for grounding, we have found that atomistic characterization of the implanted materials yields only qualitative information about the process. We show that Raman spectroscopy is a powerful tool to evaluate the ion-irradiation outcomes at while photoluminescence provides information about the electronic properties of the implanted materials. In combination with the density functional theory based ab-initio calculations, it is possible to relate these properties to the specific ion irradiation-introduced defects. Finally, we will complement the summary of our work with the description of the remaining challenges and opportunities.

NOTES

INVITED LECTURE

S3-IL7

Current state-of-the-art characterization techniques for probing polymers as electrode materials of energy storage smart windows: a case study

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Nowadays, electrochromic devices are largely investigated for applications in energy saving smart windows and displays for automobiles, airplanes, or buildings due to their ability to switch between a highly sunlight transmissive state and a colored state (that absorbs visible light), or between two colored states. One of the most important components of these devices is the electrochromic material as typical smart material responding to electrical current stimulus. Recently, electrochromic devices were endowed with energy storage functions, paving the way towards development of energy storage smart windows (ESSWs), which emerged as energy saving and multifunctional windows. ESSWs switch optical states and store redox energy in a single device based on the synergism between the electrochromic and capacitive principles of the electrode materials [1]. Polymers, either conjugated or non-conjugated are promising electrode candidates for this application due to their great advantages of color tuning under electrical bias, fast switching time, and low operating voltage. Only few polymers were tested in this regard, mainly conjugated polymers like polyanilines or polythiophenes. Recently, non-conjugated triarylamine-based polyamides were highlighted as electrode materials for ESSWs, with both color changes and charge–discharge functions [2,3]. Thus, it was demonstrated that non-conjugated polymers bearing electroactive units are also suitable candidates for use in ESSWs.

Along these lines, we have designed and synthesized a novel non-conjugated polymer containing multiple electroactive units with the aim to meet the challenges associated with its further use in ESSW applications. Several characterization methods, e.g. NMR, FTIR, UV-Vis and fluorescence spectroscopies, thermal analysis and cyclic voltammetry were primarily involved to demonstrate the polymer structure and explore its physico-chemical conduct relevant for the envisaged usage. Spectro-electrochemical profiles were further generated by coupling UV-Vis absorption spectroscopy with cyclic voltammetry and, in conjunction with chronoamperometry, were exploited to evidence the electrochromic performance of the polymer. The energy storage capability was also evaluated on the basis of the galvanostatic charge-discharge investigations performed by chronopotentiometry. Finally, the polymer was tested in the ESSW prototype configuration and the main parameters were collected to discuss the device performance.

Acknowledgements:

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References:

[1] M. Han, C. H. Cho, H. Jang, E. Kim, J. Mater. Chem. A 9 (2021) 16016–16027.
[2] C. P. Constantin, M. Balan-Porcarasu, G. Lisa, J. Energy Chem. 91 (2024) 433–452.
[3] Y. J. Shao, T. C. Yen, C. C. Hu, G. S. Liou, J. Mater. Chem. A 11 (2023) 1877–1885.

NOTES

INVITED LECTURE

S3-IL8

Structural characterization of nano-scaled materials using X-ray scattering techniques

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Nano-scaled materials play a crucial role in various applications, including coatings, paints, cosmetics, ceramics, polymers, catalysis, batteries, and drug delivery. The performance characteristics of nanoparticles are significantly influenced by their size distribution, specific surface area, and degree of dispersion. Similarly, in porous materials containing nanosized pores (used in delivery systems, separation processes, or catalysis), pore size distribution and specific surface area are critical quality parameters. Therefore, precise control and quality assessment of these properties are essential.

However, as materials shrink below 100 nm, the task of characterization becomes increasingly challenging using conventional experimental methods. X-rays, with a wavelength on the order of 1 Å, are commonly employed in diffraction experiments to analyze crystalline materials at atomic resolution. Powder diffraction enables both qualitative and quantitative analysis of crystalline phases, as well as the determination of crystallite size and interatomic distances (PDF).

Expanding the scope of X-ray scattering techniques to a wide q-range allows for the characterization of (nano-)materials across different length scales, from sub-Angstrom dimensions up to over 1000 nm. When performing wide-angle X-ray diffraction (XRD) measurements at very small angles, the electron density distribution is probed on nanometer-length scales. The small-angle X-ray scattering (SAXS) technique is particularly well-suited for the structural characterization of nano-scaled materials. It provides valuable insights into nanoparticle and pore size analysis, as well as specific surface area determination. Notably, crystallite size and particle size are distinct parameters, and SAXS, PDF, and computed tomography (CT) yield complementary structural information.

In summary, X-ray scattering techniques offer a powerful toolkit for investigating nano-scaled materials, enabling researchers to explore their structural properties across a wide range of length scales. These methods play a pivotal role in advancing our understanding of nanomaterials and optimizing their performance in various applications.

NOTES

INVITED LECTURE

S4-IL1

Able to take the heat? – Ferroelectric oxides in electrocaloric applications

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A considerable amount of the energy expenditure – and as a consequence also of the carbon footprint – of modern society is spent on thermal management, in the form of both heating and cooling. Most cooling devices are based on vapor compression technology, using hydrofluorocarbon refrigerants that have become a significant contributor to atmospheric greenhouse gas emissions. In addition, compressor-type refrigerators are not arbitrarily scalable to small size. Caloric materials, in which a degree of order can be controlled by an external variable such as a mechanical stress, magnetic or electric field, appear as a promising alternative, though they have not yet reached commercial use.

This presentation looks at the electrocaloric properties of perovskite-structured ferroelectric oxides. The focus is on two representative systems: lead scandium tantalate ($Pb[Sc1/2Ta1/2]O_3$, PST), which is attractive due to its Curie temperature close to room temperature, and barium titanate ($BaTiO_3$, BTO), which has the advantage of being lead-free and very versatile in terms of doping elements. Starting with solution-deposited thin films as model examples, the effect of B-site ordering in PST on the dielectric properties, phase transition and low-field domain response is investigated. On this basis, the field-induced temperature change, deduced indirectly from polarization P – electric field E loop measurements, is discussed, and the effectiveness of the electrocaloric response is evaluated at different temperatures.

While thin films make good model systems, their practical use is limited, as the thermal power associated with their temperature variation is too low due to their low mass. The next step is therefore based on the investigation of bulk ceramic materials. The differences in phase transition behavior as evidenced in dielectric spectroscopy between thin films and bulk systems is analyzed. A comparison of the indirect determination of electrocaloric temperature change from P(E) loops with direct temperature measurements using an infrared camera reveals the level of reliability of the indirect approach.

In a last step, a working model of an electrocaloric heat pump is presented. Based on multilayer capacitors of PST, the regenerator reaches a total temperature span of more than 20 K and a cooling power above 4 W. It is shown that, while a material with a high electrocaloric temperature change under field is of course advantageous, there are also other factors that need to be considered; it is not always the material with the highest temperature change that is most promising for applications. This allows an outlook on the future of ferroelectric electrocalorics not only for refrigeration, but also for heating applications.

NOTES

INVITED LECTURE

S4-IL2

Phase change materials for reconfigurable terahertz (meta) devices: integration and challenges

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Phase change materials or PCMs chalcogenides (GeTe, $Ge_2Sb_2Te_5$, Sb_2Te, …) have been successfully studied as agile elements in applications such as optical or electronic memories (rewritable optical disks, non-volatile memories etc.) [1,2]. They also show remarkable performance in the high frequency range - microwaves, millimeter waves and terahertz (THz), due to the ability to change their electrical and optical properties under electrical or optical stimuli between an amorphous/ insulating state (transparent in THz), and a crystalline/ conductive state which is blocking the propagation of THz waves [3, 4]. The non-volatile or bi-stable nature of the phase change is a key advantage of these technologies over conventional switching solutions at high frequencies, as the switching functions incorporating PCMs do not require a permanent bias or optical stimulus to maintain a device in a specifically prepared state. We present our research on the elaboration by magnetron sputtering of PCM thin films and their structural characterization (X-ray diffraction, Raman spectroscopy) as well as the evaluation of their electrical and optical/THz properties during the amorphous-crystalline phase change, thermally or optically induced, using very short UV and visible laser pulses (248 nm and 532 nm).

We have developed several approaches enabling fast, reversible optical control over large areas of the two different states of GeTe and have evaluated the phase change performance of these thin films in the terahertz domain using time domain spectroscopy (THz-TDS). The excellent contrast in THz properties of GeTe between the two states, was also used to demonstrate the integration of the material as agile elements in frequency reconfigurable metasurfaces or all-GeTe THz polarizers with broadband responses and very good performance [4].

By combining THz device design techniques with the unique properties of these materials, we have experimentally confirmed the feasibility of chalcogenide PCMs integration for reconfigurable THz metamaterials or spatially- coded metasurfaces allowing frequency or propagation direction control of incident THz waves.

This versatile and flexible approach based on non-volatile, optically controlled and multi-operational devices incorporating chalcogenides is expected to generate exciting developments in the millimeter wave and THz domains and anticipates novel programmable (meta)surfaces with multifunctional capabilities for electromagnetic wave manipulation.

References:

[1] M. Wuttig, N. Yamada, Nat. Mater 6 11 (2007) 824–832.
[2] S. Raoux, F. Xiong, M. Wuttig, E. Pop, MRS Bull. 39, 8, (2014) 703–710.
[3] R. Carrizales-Juarez, L. Huitema, D. Passerieux, P. Daquin and A. Crunteanu "Dielectric Properties of Phase Change Thin Films at Millimeter-Waves", IEEE Transactions on Microwave Theory and Techniques, (2023).
[4] M. Pinaud, G. Humbert, S. Engelbrecht, L. Merlat, B. Fischer, A. Crunteanu, ACS Photonics 8 (2021) 3272.

NOTES

INVITED LECTURE

S4-IL3

Micro/nanopatterning of conductive polymers for advanced biointerfaces

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Conductive polymers (CPs) and poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) in particular have emerged as promising materials for biomedical applications, including neurotechnological ones, due to their unique properties, namely mixed ion-electronic conduction, high processability in water and biocompatibility, and low impedance [1]. In this talk, I will show the possibility of exploiting both the conductivity and micro/nanopatterning of PEDOT:PSS to promote neuronal development in vitro and to fabricate highly flexible functional neural interfaces for brain recording. In particular, I will describe the design of PEDOT:PSS substrates that exhibit nanomodulated surface topography that can promote neuronal proliferation and differentiation and guide neurite elongation, especially under electrical stimulation [2]. These features are highly desired to promote neural tissue repair in cases of trauma and diseases of central and peripheral nerve tissue. Then, I will report on the fabrication of ultra-flexible PDMS-based µEcoG multi-electrode arrays (MEAs), where the integration of 3D micrometric pillars of PEDOT:PSS [3] allows for the achievement of ultra-low impedance and high softness of the elecrodes. These micropatterned MEAs have been shown to correctly record somatosensory evoked potentials (SEPs) in rat model with a high signal-to-noise ratio (SNR), confirming the advantages of CP micropatterning in the field of neural recording.

References:
[1] M. Bianchi, et al., Advanced Science 9 (2022) 2104701.
[2] M. Bianchi, et al., ACS Applied Materials and Interfaces 15 (2023) 59224–59235.
[3] A. Lunghi, et al., Advanced Materials Interfaces 9 (2022) 2200709.

NOTES

INVITED LECTURE

S4-IL4

From stagnation to success: recent breakthroughs in kesterite solar cell technology for indoor photovoltaics

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After a decade of performance stagnation of Kesterite solar cells, recent breakthroughs in the materials deposition offering a high degree of control in elemental oxidation state have permitted to bring back this technology as a strong contender in the landscape of thin film photovoltaic materials. In the meantime, the emergence of the Internet of Things and the necessity to power autonomous sensors creates a need to exploit indoor illumination. Indoor Photovoltaics is becoming a new Eldorado for photovoltaic materials with bandgaps above 1.5 eV, owing to a better spectral matching to the typical LED indoor light permitting single junction conversion efficiencies above 30%. The Kesterite family of absorber, with a bandgap tunable all the way up to 2.0 eV, retains strong assets in terms of materials availability and low toxicity, and the recent performance progress is an opportunity for this technology to finally transition from the laboratory to industrial application.

In this presentation, we will in a first part detail the experimental conditions and methods which made possible the recent breakthroughs in the field of Kesterite, we will particularly emphasis the agility of the solution-based methods initially developed at Nanjing University of Post and Telecommunications and more recently refined at the Polytechnic University of Catalonia (beyond 14% AM1.5 efficiency). This will be supported by quantitative numerical modelling providing improvement pathways and application perspectives for tandem designs.

In a second part, we will present recent results of Kesterite solar cells in indoor conditions and compare those results with other technologies, such as CIGS, Sb_2S_3, CdTe, and organic. This work will also be supported by a strong background of device modelling explaining the interplay between illumination spectrum, low injection conditions and photovoltaic conversion performance.

In a third part, we will veer towards the characterization aspect of this work. Indeed, no standard of indoor PV characterization currently exists, and we will provide arguments as to why such standard shouldn't be pursued and instead propose an easy-to-implement characterization method, applicable to the vast majority of PV-oriented groups, and providing a more relevant set of figures of merit incorporating the variability of indoor light, including both source incident power and temperature.

This presentation aims to offer a comprehensive overview of the recent breakthroughs in Kesterite solar cell technology, their suitability for indoor photovoltaics, and the development of experimental methods and characterization techniques to facilitate their evaluation by the PV research community.

NOTES

INVITED LECTURE

S4-IL5

Photo-sensitive azo-based small molecule switches

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Light sensitive molecules that are able to display multiple states due to reversible change of structure are usually called photoswitches [1]. Azobenzene is the most representative example of photoswitch which however, display a series of drawbacks, such as incomplete conversion between the isomers or rather short half-life of the least stable isomer. (Hetero)arylazo compounds [2] emerged as a promising alternative to azobenzene derivatives, resulted from replacing a phenyl ring with a heterocycle. This provides a very large number of possibilities to explore their structures, properties and mechanisms of actions, considering particularity of each heterocycle that brings different properties and open the way to a wide variety of applications.
This talk refers to novel (hetero)arylazo compounds involving various azole moieties (i.e. 1,3,4-oxadiazole [3], 1,3,4-thiadiazole, pyrazole [4]) from synthetic challenges to investigation of main parameters that characterize a photoswitch. Our results indicated surprising behavior of the compounds with respect to previously reported structures, with improvements in band separation or thermal stability.

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References:

[1] D. Bleger, S. Hecht, Angew. Chem. Int. Ed. 54 (2015) 11338–11349.
[2] S. Crespi, et al., Nat. Rev. Chem. 3 (2019) 133–146.
[3] A.F. Dobre, et al., ChemPlusChem 89 (2024) e202300504.
[4] B.C. Enache, et al., ACS Omega 7 (2022) 39122–39135.

NOTES

INVITED LECTURE

S4-IL6

Can we generate, tune or transfer CHIRALITY?

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One of our first experiences in life is the observation that our two hands are similar but not identical. If we mirror the left hand, it appears to be identical with the right hand, and viceversa. Objects which are distinct from, that is, not superimposable onto their mirror image, such as left hand and right hand, are said to be chiral.The concept of chirality is both simple and complex and it has fascinated not only scientists, but also philosophers and artists. Nowadays, chirality plays an important role in cutting-edge research in chemistry, biochemistry, physics, mathematics, medicine.

In this seminar, we will give a general introduction to chirality and its multidisciplinary aspects, with special focus on materials science. Chiral materials show unique features: the intrinsic non-centrosymmetry leads to optical rotation, circular dichroism, second-harmonic generation, piezoelectricity, pyroelectricity, ferroelectricity. We will discuss the intriguing interplay between chirality and physical properties in innovative materials, ranging from twisted bilayers to chiral hybrid organic-inorganic metal halides.

References:

[1] K. Yananose, et al., Phys. Rev. B. 104 (2021) 075407.
[2] K. Yananose, et al., Phys. Rev. B. 106 (2022) 184408.
[3] J.J. Aucar, A. Stroppa, G.A. Aucar, J. Phys. Chem. Lett. 15 (2024) 234.
[4] A. Stroppa et al., "Chiral multiferroicity in two-dimensional hybrid organic-inorganic perovskites", submitted.
[5] https://video.cnr.it/w/jtBG5CQfnxRNYZY42r759B?start=4s.

NOTES

INVITED LECTURE

S4-IL7

Chirality Induced Spin Selectivity (CISS) effect with helicene and tetrathiafulvalene derivatives

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A sustainable future requires highly efficient energy conversion and storage processes, where electrocatalysis plays a crucial role. The activity of an electrocatalyst is governed by the binding energy towards the reaction intermediates, while the scaling relationships prevent the improvement of a catalytic system over its volcano-plot limits. To overcome these limitations, unconventional methods that are not fully determined by the surface binding energy can be helpful. In this respect, thiadiazole-[7] helicene and bis(thiadiazole)-[8] helicene have been used to boost the oxygen evolution reaction (OER) by up to ca. 130 % (at the potential of 1.65 V vs. RHE) at state-of-the-art 2D Ni- and NiFe-based catalysts via the CISS effect (Nat. Commun. 2022, 13, 3356). Our results show that the chirality of the helicene molecules is accountable for a great enhancement in the activity of state-of-the-art OER catalysts. The enhancement is related to the electron spin polarization at the catalyst surface. The comparison of different electrode configurations provides a clear guideline for optimizing the enhancement (J. Chem. Phys. 2024, 160, 111103). In this contribution we will discuss as well evidences for the occurrence of the CISS effect in chiral tetrathiafulvalenes (TTF) (J. Chem. Phys. 2023, 159, 204706) and in [6]helicene-bis(thiol) through single molecule break junction.

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NOTES

INVITED LECTURE

S4-IL8

Capacitive and inductive effects in perovskite solar cells

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In the last few years the perovskite solar cells (PSCs) have shown an impressive development in terms of power conversion efficiencies. However, the stability of the PSCs is one of the most problematic issues, which still needs to be addressed. To a large extent this is due to ion migration, which is evidenced in the hysteretic effects and also in the huge apparent capacitive and inductive effects.

In Ref. [1] we introduced an equivalent circuit, which consistently explains the features in the dynamic J-V characteristics, like the normal and inverted hysteresis, the current bump in the reverse scan following a positive voltage pre-poling, as well as the peculiar capacitive and inductive effects visible in the impedance spectroscopy. Our model is based on the key assumption of ion-modulated recombination current. Here, we discuss the different roles of ionic charge accumulation and ionic charge current in reproducing capacitive and inductive effects, in close connection with the physical processes leading to photo-generated carrier recombination. The simulations are supported by experimental impedance spectroscopy data. Our approach also outlines a possible investigation route of ion migration, which aims to a more robust design of the PSCs.

Reference:

[1] N. Filipoiu, et al., Phys. Rev. Appl. 18 (2022) 064087.

NOTES

INVITED LECTURE

S4-IL9

Universal correlation between the electromagnetic interference shielding effectiveness of composite materials and their electrical properties

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With the tremendous technological developments related to the accelerated growth in the field of telecommunications, our contemporary society is increasingly facing the problem of electromagnetic pollution. The electromagnetic pollution, expected to grow even faster in the coming years, leads to electromagnetic interference phenomena that disturb the correct functioning of instruments and systems, posing thereby an important risk to industrial applications and human being. Developing technological solutions and materials for protecting instruments and systems from electromagnetic interference phenomena becomes thus a major challenge in our society. In the current work, the electromagnetic interference shielding properties and the electrical properties of poly (methylmethacrylate) based composite materials prepared using different types of fillers (carbon nanotubes, carbon black, silver coated glass microfibers) have been investigated in a broad frequency range. To this purpose, several experimental techniques have been employed (Fig. 1): Broadband Dielectric Spectroscopy (between 1 Hz and 10 MHz), coaxial cell method (between 50 kHz and 1 GHz) and the waveguide method (in the X-band: 8.0–12.0 GHz and in the Ku-band: 8.0–12.0 GHz).

By combining a theoretical and an experimental analysis we show that, irrespective of the nature of the conductive material (carbon based or metallic), the correlation between the electromagnetic shielding effectiveness, electrical conductivity and sample thickness follows a universal behavior, all experimental points falling onto a single universal curve predicted by our theoretical analysis. This is demonstrated not only for our own experimental results, but also for numerous experimental data reported in the scientific literature where other types of polymer matrices and other types of fillers have been investigated. The universal relationship found in our study opens the perspective of a precise predictive determination of the electromagnetic interference shielding effectiveness of composite materials based exclusively on their electrical properties.

References:
[1] H. Lecocq, et al., Composites Part B 189 (2020) 107866.
[2] C. Retailleau, et al., Composites Science and Technology 221 (2022) 109351.
[3] C. Retailleau, et al., A. Serghei, Macromol. Sci. Eng. 307 (2022) 2100759.
[4] H. Lecocq, et al., Polymers 246 (2022) 124740.

NOTES

ORAL PRESENTATIONS

(OP)

ORAL PRESENTATION

S1-OP1

Local vs. macroscopic properties of porous $BaTiO_3$ ceramics based on 3D reconstructed ceramic microstructures

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Porous $BaTiO_3$ ferroelectric ceramics with variable porosity level (i.e. with relative density between 74%-96%) are investigated by an experimental-numerical approach. The porous ceramics present anisotropy as derived from the deformation of sacrificial soft polymeric additives (PMMA spheres) during the pressing step [1]. 3D micro X-ray computed tomography experimental data with specific numerical procedures have been firstly used to reconstruct the ceramic 3D microstructures and to extract sample geometrical information as: pore size distribution, shape and tortuosity. These 3D microstructures have been employed as input in FEM-based models, in order to determine the local electric field and potential distributions inside the ceramic body [2]. The final aim is to evaluate the low field effective permittivity and high field ferroelectric switching P(E) and tunability responses as a function of porosity and applied field direction. The effective permittivity is estimated by computing the total electrostatic energy of the discretized system. The polarisation-field response is calculated by using a Preisach model for describing the switching properties of the dense ceramic component under the specific local field of each element. Similarly, the tunability response is computed by using a Johnson approach to describe the nonlinear dielectric response of the dense ceramic component. The resulted dielectric and ferroelectric properties derived by using this procedure are discussed in comparison with the experimentally determined ones. Piezoelectric calculations for porous ceramics are more complicated for real 3D microstructures due to the tensorial nature of this phenomenon and involve higher computational resources [3]. New approaches are currently developed for this task. The present study demonstrates the usefulness of analyses and simulations of properties at different length scales based on real 3D microstructures for completing the understanding of the complex relationship between composition – microstructure – local/macroscopic properties and pave the way of development of new tools for material design of porous or composite multi-materials.

References:

[1] R.S. Stirbu, et al., Materials 15, (2022) 6839.
[2] L. Padurariu, et al., Acta Materialia, 255 (2023) 119084.
[3] R.S. Stirbu, L. Mitoseriu, Computational Materials Science 232 (2024) 112633.

NOTES

ORAL PRESENTATION

S1-OP2

A convenient synthesis of $BaZrS_3$, $BaHfS_3$ and their solid solutions at moderate temperature

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Despite the advantages offered by inorganic chalcogenide perovskites such as $BaZrS_3$ and $BaHfS_3$ (*e.g.*, excellent thermal and chemical stability and environmental sustainability) the perspectives for their implementation in real devices are hindered by the harsh conditions required for the synthesis. Unlike hybrid perovskites, $BaZrS_3$ and similar chalcogenides cannot be prepared by low-temperature solution methods and most of the synthetic strategies proposed up to now for their preparation require extremely high temperatures (up to 1100 oC) and long reaction times and involve use of very hazardous reagents such as H_2S and CS_2.
In this work, a straightforward synthesis of BaZrS3 and $BaHfS_3$ is described [1]. The temperature employed in the present method (500 °C) is lower than in most of the previously reported ones [2] and pure crystalline materials are obtained after only several hours reaction times. Moreover, given the low temperature, the synthesis can be carried out in flame-sealed borosilicate glass ampoules, and it uses exclusively BaS, the transition metal (Zr or Hf) and S, mixed in a 1:1:3 ratio, without the need of catalysts or very expensive binary sulfides ZrS_2 and HfS_2. The same procedure was successfully applied to the preparation of solid solutions, $BaHf_{1-x}Zr_xS_3$, of the above-mentioned perovskites, obtained as single-phase crystalline solids, showing a complete miscibility of the two substances in the entire range of composition. All the synthesized materials were characterized by powder XRD and diffuse reflectance UV-visible spectroscopy and a linear variation of their structural and optical properties, namely unit cell volume and band gap value, was found, showing advantageous tunability for these chalcogenide semiconductors.

References:

[1] L. Romagnoli, et al., J. Am. Ceram. Soc. 107 (2024) 698–703.
[2] K.V. Sopiha, et al., Adv. Optical Mater. 10 (2022) 2101704.

NOTES

ORAL PRESENTATION

S1-OP3

Non-Arrhenius anomalies and large polaron tunnelling mechanisms in NaSICON superionic ceramic conductors

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Less constrained by bandwidth limitations and sampling scarcity, broadband profiling in a wide temperature range, starting at the cryogenic threshold at −150 °C and extending to 200 °C, can be used to derive parameters of minimal variance for the Jonscher power law for ionic conductivity; these are employed to model the superionic regime over elevated temperatures and frequencies beyond the limits accessed by contemporary electrochemical impedance spectroscopy (EIS) equipment. We apply this technique to non-stoichiometric NaSICON based on the canonical NZSP formula with 5% excess sodium, synthesized by an augmented solid-state reaction (SSR) method. We thoroughly analyse broadband conductivity, dielectric permittivity, and electric modulus data over the extended temperature range. Activation energy anomalies and scaling distortions inherent to the Arrhenius approximation are investigated, and an alternative formulation based on linearized difference equations is proposed to remedy these issues. With Cole–Cole analysis establishing non-Debye relaxation behaviour, dissipation analysis is employed to identify relaxation bands used for extracting initial condition parameters for the Jonscher power law. Finally, simulations of the AC dispersion region at high temperatures and frequencies suggest the dominance of polaron tunnelling mechanisms instead of the classical ion hopping mechanism previously assumed for NaSICON.

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ORAL PRESENTATION

S1-OP4

Vortex dynamics in some representative Iron-based superconducting single crystals

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The discovery of iron-based superconductors (IBS) La($O_{1-x}Fe_x$)FeAs, (x = 0.05-0.12) with a critical temperature Tc = 26 K, with unique superconducting mechanism and potential of use in various applications led to a world-wide effort in the discovery and comprehensive studies of this new class of superconducting materials. Up to now there are literally thousands of possible chemical compositions and doping levels of various IBS, of different types of crystalline structure. Lately, superconductors based on $AEFe_2As_2$ (AE being alkali-earth metal Ca, Sr, Ba) parent compound, the so-called 122 systems, became the most popular materials for both physical explorations and wire applications because of their Tc as high as 38 K, very high upper critical fields and low anisotropies, attracting substantial attention in comparison with other IBSs that have been reported in the literature. This is mainly due to the fact that in the 122 system, relatively large single crystals were relatively easy to grow using the self-flux technique. Superconductivity in $AEFe_2As_2$ is primarily induced by alkali metal (A = Na, K, Rb, Cs) substitution at AE sites. However, this type of charge doping creates strong scattering potentials that affect superconducting properties such as the vortex pinning, the upper critical field, and even the superconducting gap symmetry. Another type of 122 materials are isovalently substituted compounds such as $Ba(Fe_{1-x}Ru_x)_2As_2$ and $BaFe_2(As_{1-x}P_x)_2$, which are closer to the clean limit. More recently, a new type of IBSs has been reported, having a new structure, abbreviated as AEA1144, namely CaAFe4As4 (A = K, Rb, Cs) and SrAFe4As4 (A = Rb, Cs). In these cases, because A does not mix with AE due to the large difference in atomic radii, AEA1144 crystallizes through alternate stacking of the AE and A layers across the Fe2As2 layer, changing the space group from I4/mmm to P/4 mmm, the compounds being superconductors with Tc values between 31 and 36 K. A remarkable member of the 1144 family is $EuRbFe_4As_4$, which, after a superconducting transition at about 36 K, has a magnetic transition at 15 K, hence a clear coexistence of superconductivity and magnetism. From the point of view of potential applications in high magnetic fields, the behavior of the critical current density, and the overall vortex dynamics and pinning are of paramount importance. We have used Quantum Design PPMS and SQUID MPMS systems to measure the temperature dependence of DC and multi-harmonic AC susceptibility in various DC magnetic fields, magnetization relaxation, and magnetic hysteresis loops of three types of representative IBS, $BaFe_2(As_{0.68}P_{0.32})2$ (122 system), $CaKFe_4As_4$ and $EuRbFe_4As_4$ (1144 system) single crystals. We will present the results of the above measurements, determine some important properties from such measurements and, finally, will make a comparison between the above-mentioned single crystals.

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ORAL PRESENTATION

S1-OP5

Morphology and structural properties of M-hexaferrite

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Hexagonal ferrite materials based on Ba^{2+} or Sr^{2+} have attracted attention in practical applications, due to their remarkable physical properties, especially ferroelectric and ferromagnetic. Layering structure P63/mmc is formed with two planes containing M^{2+} ions capping some Fe_2O_3 and FeO structures in two distinguished sites: A-site with tetrahedral symmetry dominated by Fe^{3+} ions and a combination of Fe^{2+} and Fe^{3+} in an octahedral symmetry. Magneto-optical measurements enable the identification of Fe^{2+} and Fe^{3+} of $BaFe_{12}O_{19}$ M-hexaferrite powder obtained by sol-gel processing, followed by thermal annealing at 900 C for 3 hours. The ferromagnetic phase is evidenced by the spin-majority configuration (Fe^{3+}) due to their unpaired electrons between d-d orbitals, while the Fe^{2+} in the low spin possesses diamagnetic behavior strongly dependent on the surrounded crystal field. Additionally, the irradiation with gamma rays changes the ratio between Fe^{2+}/Fe^{3+}, mainly on the surface of $BaFe_{12}O_{19}$ nanocrystals. After the gamma-irradiated $BaFe_{12}O_{19}$ powder, the thermoluminescence measurements confirm the conversion of Fe^{3+} in Fe^{2+} by electron capture, which releases a red photon during the thermally activated recombination processes. This reduction process induces the broken of some Fe^{3+}(i)-O^{2-}- Fe^{3+}(j) (j=1, 2, 3, 4, 5) and the creation of the hole centers (e.g. O^{2-} near the Fe^{3+} ion), which in turn, weakens the super exchange interactions, responsible for the magnetic properties of $BaFe_{12}O_{19}$.

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ORAL PRESENTATION

S1-OP6

A revised theory of band ferromagnetism

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Ferromagnetism in 3d metals is re-examined in a simple band model. It is firstly shown that the molecular field model cannot account for the low values of coercive field in ferromagnetic pure metals, and that the standard Stoner theory of band ferromagnetism incorrectly evaluates the total electronic energy and cannot predict reasonable Curie temperatures. A new simple band model for magnetism is formulated, by considering the total one-electron energies in spin split subbands and not only the increase in kinetic energy at Stoner excitations. This yields a criterion for ferromagnetism even in absence of a stabilizing Hubbard term, involving only the density of states (DOS) at the Fermi level, its derivative and the filling of the 3d band. In a simplified picture, when the derivative of the one-electron paramagnetic DOS is negative, spin asymmetry occurs in a natural way up to the complete filling of the majority spin subband. By introducing a double-peaked DOS, one may explain the occurrence of ferromagnetism in bcc Fe, hcp-fcc Co and fcc Ni, the stabilization of fcc-hcp or bcc structures across all 3d elements, the occurrence of antiferromagnetism in chromium, and derive reasonable Curie temperatures [1]. Another prediction is related to 're-entrant' ferromagnetism at very high temperatures, provided the solid survives at such temperatures. This might have applications in the origin of the geomagnetic field and will be detailed in another communication.

The actual model might be extended also to semiconductors, naturally described by a 'twin peaks' DOS where the valence band is separated from the conduction band. The situation is complicated by the fact that the valence and conduction DOS are generally not similar. As the roughest approximation, by supposing conduction and valence band described by Dirac delta functions and that after the spin polarization the majority sub-band is shifted towards lower energies up to the complete filling of the conduction band, while the minority sub-band is shifted towards higher energies up to the complete depletion of its valence band, an immediate evaluation yields that the spin polarized state is lower in energy when the Fermi energy (in the unpolarized state) is located below the middle of the bandgap, which implies an initial p doping of the semiconductor. Thus, this model may be applied also for diluted magnetic semiconductors.

Reference:

[1] C.M. Teodorescu, Res. Phys. 25 (2021) 104241.

NOTES

ORAL PRESENTATION

S1-OP7

Ternary hydroxyapatite-titania-graphene biocomposites produced by green process and their bioactivity behaviour

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The use of non-toxic, biocompatible materials is crucial for the repair and reconstruction of tissues damaged as a result of injuries. In recent years, efforts to produce with green processes have been increasing in all fields of science. In this study, sheep hydroxyapatite (SHA) produced in the laboratory was used to produce biocompatible composite materials as well as to utilize sheep bone waste. Two separate mixtures containing 95wt.% sheep hydroxyapatite-5wt.% titania-0.5wt.% graphene and 95wt.% sheep hydroxyapatite-5wt.% titania-1wt.% graphene were prepared and mixed in a jet mill for 4 hours. The press-formed samples were sintered at 3 different temperatures of 1100, 1200 and 1300 □C. The samples obtained were subjected to density measurement, compressive strength, Vickers Microhardness measurement tests. The formed phases were detected by XRD analysis and microstructure examinations were performed by SEM. Bioactivity tests were applied to the bioceramic composites that gave the best mechanical results. The composites, which were subjected to static in vitro bioactivity test during 2,3 and 4 weeks of storage in simulated body fluid, were determined to be bioactive by the dense hydroxycarbona apatite layer formed.

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ORAL PRESENTATION

S1-OP8

Cu-Zr-Al metallic glass matrix composites with in-situ precipitated phase reinforcement

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This study delves into the synthesis and characterization of Cu-Zr-Al alloys, aiming to enhance their mechanical properties through the formation of amorphous-crystalline composites. By investigating factors influencing the formation of the B_2 CuZr phase during solidification and martensitic transformation, this research may constitute the commercial potential of these materials. Various techniques, including alloy synthesis, casting, mechanical testing, and microstructural analysis, have been employed to achieve this goal. Metallic glasses hold great promise in engineering applications, offering unique properties such as high strength and corrosion resistance. However, their fragility has limited their widespread use in load-bearing scenarios. To overcome this limitation bulk metallic glass composites, with particular emphasis on Cu-Zr-Al alloys, are explored. By incorporating crystalline phases into the glassy matrix, these composites aim to combine the excellent properties of metallic glasses with the ductility of crystalline materials.

In this work we study a group of alloys, cast in an arc furnace under protective argon atmosphere, with a chemical composition of $Cu_{48}Zr_{45}Al_7$ with a diameter ranging from 5 mm up to 10 mm, ensuring the formation of the B_2 CuZr phase during solidification that transforms into B19` phase during deformation. In addition, the effect of cooling rate on the structure and properties of the composite will be examined in detail. The structures of the samples were characterized by X-ray diffraction, and the amount of crystalline precipitations was calculated using light microscopy. Uniaxial compression tests were performed to determine the compressive yield strength and compressive fracture strength. Fracture analysis via scanning electron microscopy (SEM-SE) revealed differences in fracture behavior between alloys. Additionally, differential thermal analysis (DTA) was employed to assess glass transition behavior, crystallization, melting temperatures, and providing insights into the glass-forming ability and tendency to formation of the B_2 phase during solidification.

NOTES

ORAL PRESENTATION

S1-OP9

Composite photocatalysts based on carbon structure and semiconductors obtained by recycling electronic wastes

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Recycling electronic waste (e-waste) has become a significant concern due to environmental regulations governing product disposal. E-waste, which includes items like mobile phones, alkaline and Li-ion batteries, toner cartridges, and used office paper, contains valuable resources such as metals, semiconductor oxides, magnetic oxides, and various carbon structures. There are several proposed or operational processes for recycling e-waste, each with its own advantages and disadvantages. It is crucial to optimize recycling efficiency while minimizing environmental damage. In this study, we focus on recycling ZnO-based nanostructures from spent alkaline batteries and simultaneously creating carbon-based structures from used office paper. The ultimate goal is to develop a composite that exhibits more desirable characteristics than each component taken separately. Therefore, the obtained samples were tested as photocatalysts for degrading organic compounds in wastewater. ZnO-based nanostructures were obtained from spent batteries using a mild hydrometallurgical method and annealed at various temperatures. The carbon structures were produced from used office paper through specific cleaning, activation, and calcination processes. To assess their properties, the composite samples were characterized using XRD, TEM, FTIR, UV-VIS, PL, and TGA analyses. Photocatalytic tests revealed that the carbon-based composite structures exhibit photocatalytic activity towards degrading RhB dye. These strategies are crucial for promoting clean energy and sustainable development.

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ORAL PRESENTATION

S1-OP10

Fabrication and characterization of sponge-like PDMS composites

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Water purification by using polydimethylsiloxane (PDMS) have been the subject of numerous studies due to PDMS advantages, such as easy operation, relatively low cost fabrication, reusability and high performance. PDMS is a flexible polymer with high thermal and mechanical stability, inert, non-toxic, which can be cast into molds with different geometries to obtain materials with different shapes. Moreover, its properties such as biocompatibility, low toxicity and reusability increased the interest granted to the class of silicon-based polymers used for water management technologies. A convenient method for the preparation of PDMS-based adsorbent materials with high specific surface area, such as 3D spongy structures with interconnected pores, is to use sacrificial materials that are also environmentally friendly such as sugar, salt or other materials capable of dissolving when immersed in water, thus creating pores in the material whose distribution and dimensions depend on the sacrificial matrix/template used. This method is rapid, does not require complicated synthesis steps or expensive equipment, generating the adsorbent material quickly and at low cost. However, even in this fabrication process, problems may arise regarding the elimination of the rigid sacrificial matrix from the polymer structure. In order to improve the efficiency of the purification of pollutants from wastewater, studies demonstrated how involvement of PDMS, as a host in preparation of photocatalytically-active materials in various configurations, can help to overcome limitations of powder photocatalysts and increase the efficiency of photocatalysis.

In this paper, we present our studies regarding the fabrication of sponge-like PDMS based composites obtained by incorporating photocatalysts such as TiO_2 or ZnO in order to improve the PDMS performances in water treatment. Thus, the process of pollutants' degradation is improved by avoiding the filtration and powder removal steps. The sponge like PDMS 3D-architectures will be characterized from the morphological and structural point of view and their photocatalytic properties will be presented.

NOTES

ORAL PRESENTATION

S1-OP11

Rare-earth doped GdF_3/$LiGdF_4$ nanocrystals in silica glassy nanocomposites: crystalline phase tuning and luminescence properties

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Rare-earth doped GdF_3 and $LiGdF_4$ nanocrystals embedded in SiO_2-GdF_3/$LiGdF_4$ silica glassy matrix have been prepared by controlled crystallization of the xerogel; the influence of rare-earth ion (RE =Pr, Sm, Eu, Tb, Dy, Er, Yb) and additional Li-codopant on structural (crystalline phase) and optical properties was investigated. The precipitation of RE^{3+}-doped fluoride nanocrystalline phase is the result of Gd, Li trifluoracetates thermolysis at around 300 C and is based on autocatalytic process where the second LiF metastable phase acts as a catalyst that accelerates the crystallization process.

Structural analysis of the RE^{3+}-doped glassy nanocomposite sample showed high improvement of the crystallization for Li co-doped samples (1 mol%) caused by a decrease of the energetic barrier for the nanocrystal formation. The occurrence of GdF_3 nanocrystals (tens of nm size) which are showing hexagonal or orthorhombic structure is primarily driven by the RE-ions dopant size. The crystalline lattice distortion effects are associated to the RE^{3+} incorporation in the crystalline lattice.

Under UV-light excitation at 273 nm of Gd^{3+} ions (8S7/2-6I13/2,15/2 transition), photoluminescence spectra showed characteristic RE^{3+} luminescence due to the non-radiative energy transfer between the excited Gd^{3+} and acceptor RE ions; the highest energy transfer (about 80%) was observed for Tb^{3+} and lowest (about 21%) for Sm^{3+}.

For higher Li co-doping (up to 4mol%) we observed the precipitation of the $LiGdF_4$ nanocrystals in the silica matrix and strong distortion of the crystalline lattice. Under 980 nm laser-light pumping they are showing “green” ((2H11/2, 4S3/2) -4I15/2) and “red” (4F9/2-4I15/2) up-conversion luminescence at 525, 545 and 660 nm, assigned to the Er^{3+} ions de-excitation with a signal magnitude close to the other similar glassy nanocomposites (such as RE^{3+}-doped SiO_2-CaF_2 or SiO_2-$LiYF_4$ glassy nanocomposites).

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ORAL PRESENTATION

S1-OP12

Improved thermo-physical and mechanical properties of Tungsten with dispersed nanometric ZrC particles processed by SPS and a subsequent thermo-mechanical treatment

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Tungsten materials with 20 nm ZrC dispersoids have been produced from different W powders using a mixed dc/pulsed dc SPS cycle with several steps, followed by a thermomechanical treatment using an uniaxial hot-pressing equipment. Depending on the processing route, consolidated materials with almost full densification were obtained. Long term annealing studies at 1450 °C followed by microstructural characterisation using SEM/EBSD and hardness investigations revealed a stable microstructure even for samples with low density. Thermo-physical property investigations have shown only small decreases in thermal conductivity compared to pure W and a slight increase of the thermal expansion coefficient. 3-point bending tests performed from room temperature up to 600 °C revealed different behavior depending on the initial W powder particle sizes. Specimens produced with a mixture of 75% 40 um and 25 % 900 nm W powders show an almost ductile behavior in the compressed part and trans-granular fracture in the tensile stressed part even at low temperatures pointing to a role of the ZrC dispersoids in the reduction of intergranular fracture. Specimens produced solely from 40 um W powders show a similar W trans-granular fracture at low temperatures and a clear ductile behavior from 300 °C upwards. Oppositely, similar materials produced with only 2 um W powders show brittle fracture even at 600 °C.

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ORAL PRESENTATION

S1-OP13

Numerical simulations of unsteady thermal and oxygen transport in a Czochralski process for solar silicon growth

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The ultimate potential of each material is limited by the presence of defects and impurities. The impurities are incorporated in melt-grown crystals at the solid-liquid interface. In the longitudinal sections of these crystals the so-called striations can be observed which reveal the pattern of the impurities incorporated in crystals and display the shape of the solid-liquid interface. In general, the occurrence of striations in melt growth is mainly caused by fluctuations of the growth rate V, which influences the incorporation of the solute according to the segregation effect [1]. Unsteady heat transfer in melt growth generates fluctuations of the growth rates. Therefore, it is expected that striations pattern to be influenced not only by the impurity distribution in the melt but also by the temperature fluctuations.

Melt convection is acknowledged to be a very important factor in the field of crystal growth. It can be stated that the control of convective transport is one of the key parameters for the control of material properties and crystal yield in industrial production of Cz-silicon crystals. Convective flows are contributing to the heat transfer and thus controlling the rate of solidification, which is very high (tens of mm/h) in the case of silicon for photovoltaic applications in comparison with the case of silicon for electronic applications.

The resulting temperature field in the vicinity of the solid-liquid interface is affecting its shape and therefore the generation of thermal stress and the formation of dislocations. Convection also controls the species/impurity transport in the melt. It affects the dissolution rate of crucible materials, the entry and evaporation of impurities from, respectively to, the gas phase via the melt free surface. Furthermore, in a complex interaction of both heat and species transport, convection strongly influences the morphology and stability of the solid-liquid interface.

It is the aim of this work to perform numerical simulations, using STHAMAS 3D software to predict the temperature and oxygen concentration fluctuation in the melt, induced by natural convection and forced convection due to crucible and crystal rotation in a 200 mm Cz-Si process for different growth conditions. Furthermore, different types of crucible rotation schemes (counter or isorotation, Accelerated Crucible Rotation Technique (ACRT) will be consider to study their influences on the temperature and oxygen distribution and time oscillations.

References:

[1] J. Friedrich, W. von Amon, G. Mueller, Handbook of Crystal Growth: Bulk Crystal Growth, pp. 46–98, Elsevier, (2014).

NOTES

ORAL PRESENTATION

S1-OP14

Progress in the growth of crystals for optical and thermal barrier coating applications

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Rare earth silicates are an interesting class of materials owing their potential for optical (laser diodes, scintillators) and environmental barrier coating (EBC) applications. One of the major difficulties encountered in the synthesis and study of these systems is due to the existence of a relatively large number of chemical phases (e.g. R_2SiO_5, $R_2Si_2O_7$, $R_{4.67}(SiO_4)_3O$) and polymorphism possible at ambient pressure, i.e. depending on the nature of the lanthanide ion and temperature, R_2SiO_5 crystallizes in 2 crystal-types, whereas $R_2Si_2O_7$ forms 7 crystal structures. Moreover, there is an overlap of the thermodynamic stability ranges of the different polymorphs and/or chemical phases, thus hindering the synthesis of pure phase ceramic materials by conventional solid state reaction. To overcome these drawbacks and study the intrinsic properties of these systems, one can attempt to prepare these materials in crystal form.

Some members of the $R_2Si_2O_7$ family were previously grown by the floating zone method using conventional halogen-lamp-heated furnaces. Nevertheless, the boules obtained were comprised of multi grains, had thermally generated cracks and the single crystals isolated from the boule were too small to study extensively these materials. The growth of some members of the R_2SiO_5 family has recently seen a renewed interested due to advances in the floating zone method with the development of laser-diode-heated floating zone furnaces. However, some of the crystals obtained were comprised of multi grains, opaque and had thermally generated cracks.

Here, we present the results of our investigations to optimize the synthesis and crystal growth conditions of R_2SiO_5 (R = Dy, Ho and Er), and discuss the properties of these materials [1]. Our study proves the complementarity to the conventional halogen-lamp-heated and laser-diode-heated floating zone furnaces. Our attempts to grow members of the R_2SiO_5 series using conventional halogen-lamp-heated furnaces failed to yield any crystals, i.e. the desired chemical phase appears to melt incongruently, and the melt was found to be composed of other chemical phases than the desired one. Alternatively using a laser-diode-heated furnace we successfully prepared large, high quality, crack-free and pure phase single crystals of R_2SiO_5. Our results show that the different thermal profile of the heated zone compared with conventional halogen heated floating zone furnace is crucial in the stabilization of the R_2SiO_5 phase and our findings could be extended to other families of rare earth silicates. This progress is crucial for the study of the intrinsic structural, chemical and physical properties of these materials which will open the route for improving the properties of these materials for applications.

Reference:

[1] V.C. Ciomaga Hatnean, et al., Crystals 13 (2023)1687.

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ORAL PRESENTATION

S1-OP15

Study of thermal decomposition of formamidinium tin triiodide perovskite by means of Knudsen effusion mass spectrometry

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Although metal halide perovskites are among the most promising semiconductors for solar cells, the lead-based ones, which have shown up to now the best performances, pose some concerns due to the presence of toxic Pb. This has led in the last few years to an increasing focus on lead-free perovskites, among which the tin-based ones have emerged as the most viable alternative, in terms of optoelectronic properties and element availability. In this respect, even though advances have been made in tin perovskites solar cells efficiency [1], their thermal and chemical instability is a serious issue, not less than for the Pb-based counterparts, especially considering that Sn(II) can be easily oxidized to Sn(IV), with detrimental consequences for photovoltaic devices.

However, unlike lead halide perovskites, for which thermal degradation has been extensively investigated in recent years [2,3], a detailed insight into decomposition processes occurring in Sn-based ones is still lacking. The aim of the present study is therefore to elucidate thermal decomposition of formamidinium tin triiodide, by the experimental approach applied recently to the investigation of the corresponding lead-based perovskite [4]. In particular, Knudsen effusion mass spectrometry allowed the identification of gaseous species released upon heating, in the temperature range 366–462 K, and the determination of their partial pressures. Several decomposition products originated from the organic portion of the perovskite were found in the vapor phase, similarly to what observed for formamidinium lead triiodide, namely NH3(g), HCN(g), CH4N2(g) (formamidine), H3C3N3(g), (triazine) and HI(g), indicating the following degradation pattern:

$CN_2H_5SnI_3(s) \rightleftharpoons SnI_2(s) + CN_2H_4(g) + HI(g)$

$CN_2H_5SnI_3(s) \rightleftharpoons SnI_2(s) + NH_3(g) + 1/3\ H_3C_3N_3(g) + HI(g)$

$CN_2H_5SnI_3(s) \rightleftharpoons SnI_2(s) + NH_3(g) + HCN(g) + HI(g)$

However, in striking contrast with thermal behavior of the corresponding lead perovskite, also the abundant release of tin-containing gaseous products was observed. In particular, both $SnI_2(g)$ and $SnI_4(g)$ were identified in the vapor phase, but, while the former showed vapor pressure values corresponding to those of the pure compound, indicating its formation as a solid decomposition product and subsequent sublimation, SnI4 partial pressures are significantly lower than those of $SnI_4(s)$. This suggests the presence of Sn(IV) impurities in the perovskite, rather than the formation of $SnI_4(s)$ in the solid phase, especially since SnI_4 pressures are higher in the initial phases of the experiments and gradually decrease as perovskite degradation proceeds.

References:

[1] S.M. Hasnain, Sol. Energy 262 (2023) 111825.
[2] B. Brunetti, et. al., Sci. Rep. 6 (2016) 31896.
[3] A.F. Akbulatov, et. al., Sol. Energy Mater. Sol. Cells 213 (2020) 110559.

NOTES

ORAL PRESENTATION

S1-OP16

Re-entrant ferromagnetism occuring from a simple band model as a possible origin of the geomagnetic field

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A recent theory of band ferromagnetism in 3d metals predicts 're-entrant' ferromagnetism at temperatures far above the boiling point of these metals in normal conditions [1]. Metals, and in particular iron rich alloys, are still solid at such extremal temperatures in the Earth's inner solid core. It follows that this piece of the Earth may become ferromagnetic. This hypothesis is investigated in this work in more details, by using densities of states derived by ab initio density functional theory calculations for hexagonal close-packed iron and applying the basic theory of band ferromagnetism derived in [1]. The temperature for 're-entrant' ferromagnetism increases with the pressure, ranging between about 6530 and 6640 K for pressures between 330 and 360 GPa; these temperatures are in the range of most estimates for the temperature of the inner solid core of our planet. The dimension of the ferromagnetic "innermost inner core" (IMIC) derived from the estimated Fe magnetic moment are within the dimensions of a IMIC with different anisotropy in the propagation of seismic waves. For body centered cubic Fe no 're-entrant' ferromagnetism is predicted based on the actual model. It follows that the Earth's inner solid core with hexagonal close-packed structure is the main responsible for the geomagnetic field, and also most probably the reversal of this field proceeds by simple rotation of the magnetization of this core, while keeping a non-vanishing magnetic field during the reversal. The reversal may therefore be driven by some external magnetic field, such as that generated by solar protuberances or magnetic planteoids approaching the Earth. This process of progressive reversal while keeping the magnetic field intensity constant might prevent the Earth's surface bombardment with energetic charged particles during the reversals, with beneficial effects for complex lifeforms and for mankind civilization [2]. Other information suggesting the interplay between the IMIC solidification in the Earth's center and the occurrence of sophisticated lifeforms is related to the similarity between the age of the solid core [3] and the Cambrian explosion of lifeforms, about 560 million years ago.

References:

[1] C.M. Teodorescu, Res. Phys. 25 (2021) 104241.
[2] C.M. Teodorescu, M.A. Husanu, Phys. Earth Planet. Inter. 32 (2022) 106856.
[3] R.K. Bono, et. al., Nature Geosci. 12 (2019) 143–147.

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ORAL PRESENTATION

S1-OP17

On gravity and gravitational anisotropic meta-materials

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Observation, experiment and theory had firmly established gravitational interaction as a weak effect due to nucleon spin (quark field) polarization. This is well technologically understood and controlled in NMR / nuclear magnetic imaging, but without concern to associated gravitational effects. The nuclear spin polarization effect is analogous to magnetism as an effect of electron orbital / spin polarization.

Prospects of new materials with an anisotropic response to gravitational field will be presented, both for pre-fabricated (permanent magnets) and dynamically controlled devices as well (the analog of electromagnets).

The Material Science engineers' community is invited to broaden their research in this new direction.

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ORAL PRESENTATION

S1-OP18

New workflow-based methods for material research

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To fully understand the characteristics and properties of a material a number of methods like macroscopic and nanoscopic phase analysis, chemical analysis, analysis of mechanical properties and the behavior under certain environmental conditions like temperature and stress need to be applied. This typically involved different modalities like light and electron microscopy - in 2D but also in 3D. In addition, non-destructive X-ray microscopy enables to locate regions of interest (ROIs) on the µm-scale to be then further investigated with SEM or FIB/SEM. In this talk we will show the sample centered, holistic workflow-base approach that bridges several orders of magnitude and involves different microscopy modalities.

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ORAL PRESENTATION

S2-OP1

Oxygen vacancies and applied electrical field conditioning of polar phase in hafnia nanocrystals

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Given the continuously rising global energy demands, there has been a notable surge in interest in energy harvesting technologies across both research and industry sectors. Pyroelectric energy harvesting (PEH) presents a promising avenue for diverse end-user applications, particularly in thermal sensing. This technology effectively converts abundant waste heat, emitted by various industrial processes, into electric energy. Additionally, it can harness heat from hot surfaces or gases, such as microelectronic components experiencing self-heating during operation, refrigerators generating heat that warms the surrounding air, and the heat absorbed by walls and windows of buildings during summer days. Moreover, PEH can capture the high-temperature exhaust gases produced by internal combustion engines.

The pyroelectric nature of HfO_2-based materials was first unveiled in 2015 by Hoffmann et al. and further empirically explored in few subsequent studies which underlined the good perspectives of hafnia-based materials for PEH applications.

Nano-crystalline hafnia thin film-based devices exhibited a pyroelectric effect in spite of being mainly crystallized in the non-polar monoclinic system, as the structural analyses have revealed. The pyroelectric output was linked to the positively charged oxygen vacancies present in the hafnia grains. Moreover, the capacitance variation with temperature disclosed a tetragonal-to-orthorhombic phase transition having a Curie temperature of ~200 K. The notable electrical differences recorded between hafnia grown on silicon dioxide and aluminum nitride interlayers, accounted for their dissimilar pyroelectric performance. The pyroelectric properties of hafnia-based devices were improved significantly (from 0.10 $\mu Cm^{-2}K^{-1}$ to 0.17 $\mu Cm^{-2}K^{-1}$) by using the aluminum nitride interlayer, as consequence of its polar nature and its capability to induce more oxygen vacancies in hafnia.

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ORAL PRESENTATION

S2-OP2

Some contributions to metal oxide-based multifunctional hybrid thin films for transparent and flexible electronics by bottom-up approach

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Bottom-up nanotechnologies have enabled low-cost, large-area transparent and flexible thin-film transistors below 200 °C on different substrates. Integrating transparent thin film transistors with semiconductor metal oxide channel (MOTFT) into electronics led to the development of transparent and flexible electronic (TFE) applications. Printing technologies of multifunctional thin films over flexible large areas of low-voltage operation of organic field effect transistors (OFETs) enabled devices suitable for stretchable and wearable electronics. Integrating hybrid nanomaterials based on metal oxide, quantum dots, metals, polyelectrolytes, or organic semiconducting polymers resulted in new flexible and stretchable electronics (FSE). Bidirectional flexible large-area organic circuits consisting of active matrix flexible and stretchable sensors with low power consumption and reduced connecting wiring ("artificial skin") are among the essential applications of FES.

This presentation highlights some of our relevant contributions to obtaining ZnO-based multifunctional thin films for transparent&flexible electronics, *i.e.*, Al:ZnO TCO [1], ZnO/SiO_2 [2], and hybrid ZnO/PMMA, ZnO/Chitosan/PMMA, and Ag:ZnO/Chitosan/PMMA [3], by (modified) sol-gel methods. All the components integrated into the hybrid thin films (Ag, ZnO, Chitosan, and PMMA) demonstrated the capabilities to act as multifunctional (nano)material in various biocompatible electronic devices as (bio)sensors and wearable electronic patches. ZnO-PMMA hybrids were proposed for nanodielectric. Ag prevents electron-hole recombination, increasing the electrical conductivity, photocatalytic and antimicrobial activities of Ag:ZnO nanoparticles. In hybrid flexible dielectric films for advanced electronics, Ag, well-known as antimicrobial agent, can lead to new frontier applications. By protonic electrical conduction, the flexible biocompatible and biodegradable chitosan demonstrated effective hybrid gate dielectric in TFTs and OTFTs.

References:

[1] V. Musat, et al., Surf. Coat. Technol. 180–181 (2004) 659–662.
[2] V. Musat, et al., Thin Solid Films 516 (2008) 1512–1515.

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ORAL PRESENTATION

S2-OP3

Thin film cupric oxide as absorbing layer for solar cells in space applications

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Copper oxides, are known as p-type semiconductor materials, that characterize with high light absorption, rendering them highly desirable candidates as absorber layers within thin film solar cell architectures. Typically paired with n-type materials such as ZnO or TiO_2, copper oxides offer a compelling alternative to traditional thin film photovoltaic technologies like CdTe and CIGS, primarily due to their non-toxicity and the abundance of their constituent raw materials. Moreover, their production entails less energy consumption compared to the manufacturing processes associated with crystalline silicon, thus positioning them favorably in the realm of sustainable energy technologies. In contrast to the promising perovskite and organic-based solar cells, which confront challenges related to stability, cupric oxide is stable among copper oxides. Beyond their application in photovoltaics, copper oxides find utility in diverse fields, including photocatalysis and sensor technologies.

Given the critical role of photovoltaic systems in powering space missions, it becomes imperative to assess the resilience of cupric oxide thin films to the deleterious effects of proton irradiation, particularly in environments characterized at the low earth orbit missions. The utilization of thin film photovoltaics not only promises mass reduction but also addresses the pressing economic concerns associated with the transportation of solar cells into outer space, thereby facilitating the realization of sustainable and cost-effective energy solutions for extraterrestrial endeavors.

We employed the reactive magnetron sputtering technique to deposit CuO thin films onto glass slab substrates, the process was controlled to achieve thickness of 130 nm. Subsequently, the prepared samples were irradiated with protons possessing energy of 226 MeV and a fluence of $1x10^{11}\cdot cm^{-2}$, this experiment was performed at the Institute of Nuclear Physics in Krakow. Experimental characterization involved the assessment of absorbance using UV-Vis spectrophotometry, and refractive index along with extinction coefficient using spectroscopic. Furthermore, the determination of sheet resistivity through four-point probe measurements provided insights into the electrical conductivity of the thin films, crucial for evaluating their performance in photovoltaic applications. To comprehensively understand the structural and compositional changes induced by proton irradiation, X-ray photoelectron spectroscopy (XPS) was employed to probe alterations in the surface chemical states of copper and oxygen. The precise analysis of XPS spectra, conducted at the National Institute of Materials Physics in Magurele, facilitated the identification of irradiation-induced modifications, thereby enhancing our understanding of the material`s response to harsh radiation environments.

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ORAL PRESENTATION

S2-OP4

Chiral multiferroicity in two-dimensional hybrid organic-inorganic perovskites

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Tunable chemical compositions in hybrid organic-inorganic perovskites (HOIPs) enable the tailoring of magnetic, electric, and chiral properties, thereby affording them as a new class of chiral multiferroics. Despite the coexistence of electric and magnetic orders within HOIPs, the underlying mechanism of magnetoelectric correlation as well as its interplay with chirality transfer remains unclear. Through Landau-based symmetry mode analysis, we demonstrate that the chirality transfer, ferroelectric, and ferromagnetic orders are mutually coupled in layered multiferroic Cu-based HOIPs. We introduce a new intuitive pseudo-scalar descriptor, based on ferroelectric moment and a ferro-rotational moment, which differentiates the chirality of (R)- and (S)-HOIPs through its sign. The sign change of chirality transfer descriptor is accompanied by the synergetic switching of ferroelectric distortion, Jahn-Teller anti-ferrodistortion as well as Dzyaloshinskii-Moriya vectors, manifesting the chirality-correlated magnetoelectric coupling in HOIPs.

References:

[1] B. Sun, et al., Chem. Mater. 32 (2020) 8914.
[2] J.J. Aucar, et al., J. Phys. Chem. Lett. 15 (2024) 234.
[3] A. Stroppa, et al., Angew. Chem. Int. Ed. 50 (2011) 5847.
[4] A. Stroppa, et al., Adv. Mater. 25 (2013) 2284.
[5] A. Stroppa, et al., "Chiral multiferroicity in two-dimensional hybrid organic-inorganic perovskites", submitted.

NOTES

ORAL PRESENTATION

S2-OP5

Prediction of glass formation ability in chalcogenides using machine learning algorithms

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Due to their remarkable electrical and optical properties, chalcogenide glasses (ChGs) exhibit applications in areas such as optical fibers, solid-state batteries, thermal imaging devices, and ovonic threshold switches. Capitalizing on the recent integration of Artificial Intelligence within Materials Science, this study aims to use machine learning for the identification of new, homogeneous, and stable ChGs. To achieve reliable predictions, we collected an extensive dataset of approximately 58 000 chalcogenide compounds from the SciGlass database and employed ten machine-learning models in a binary classification framework. This selection includes eight conventional algorithms: k-nearest neighbors, random forest, extreme gradient boosting, histogram-based gradient boosting, light gradient-boosting machine, extremely randomized trees classifier (ExtraTrees), adaptive boosting of decision trees, and categorical boosting. Additionally, we trained two meta-learner models, Voting and Stacking Classifiers, which significantly improve performance metrics during testing. This research emphasizes the potential and limitations of using machine learning for glass material classification. Notably, the predictive accuracy of these models is anticipated to be most applicable to glass compositions synthesized through prevalent techniques represented within the SciGlass database. After the optimization of hyperparameters, all models demonstrated notable values for the F1-score, Matthews correlation coefficient, and the Receiver Operating Characteristic - Area Under the Curve (ROC-AUC) score metrics, which measure the model ability to distinguish between classes. Only several models exhibited an ability to extrapolate effectively to our experimental dataset of 417 thin-film compositions, not previously encountered in the collected data, prepared by magnetron sputtering. The ExtraTrees model stands out by achieving 67% accuracy and a 70% ROC-AUC score. In the methodology developed in this investigation, a comprehensive array of 324 initial candidate features was constructed for each composition to capture the influence of relevant elemental properties on glass-forming ability. Each feature vector provides a unique quantitative physico-chemical profile for a composition, based on an extensive list of elemental quantities rather than experimental synthesis methods. Proceeding with the validated models, SHAP (Shapley additive explanations) feature importance analysis was conducted to elucidate the relationships between theoretical parameters and the glass-forming ability in chalcogenide materials. This comprehensive study demonstrates the potential of machine learning in facilitating the discovery of new ChGs but also emphasizes the importance of integrating theoretical and empirical data to enhance predictive accuracy.

NOTES

ORAL PRESENTATION

S2-OP6

Physical properties of submicrometric RF-sputtered CdTe thin films for photovoltaic applications

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This study presents an in-depth analysis of cadmium telluride (CdTe) thin films deposited on p-type silicon (Si) and optical glass substrates, simultaneously, through radio frequency magnetron sputtering. Deposition processes have been run at various working powers (70, 80, 90, and 100 W), holding the substrate temperature, working pressure, and deposition time at 220 °C, 0.46 Pa, and 30 minutes, respectively. We have investigated the structural, morphological, and optical characteristics of the CdTe films using X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM), and optical spectroscopy techniques. Electrical characterization of Ag/CdTe/Al "sandwich" structures was conducted via current-voltage characteristics, revealing insights into charge transport mechanisms. Our results highlight 90W RF power as optimal for achieving high crystallinity in ~1 μm nanostructured thin films, on both p-Si and optical glass substrates. Their optical and electrical properties are suitable for absorber layers in CdTe photovoltaic cells. This research contributes valuable insights into optimizing CdTe thin film deposition techniques for enhanced photovoltaic performances of the solar cells based on very thin films of A2-B6 semiconducting compounds.

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NOTES

ORAL PRESENTATION

S2-OP7

Microscopic models of ferroelectricity in thin films and predictions of mean field theories based on them

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A simple view of ferroelectricity is proposed for a thin film with uniform polarization oriented perpendicular to its surface, starting from the assumption that this situation is always accompanied by charge accumulation in the outer metal electrodes, in the contamination layers or near surface, in the ferroelectric film itself [1]. Starting with the formula derived for an "elemental" dipole moment in the film, simple statistical mechanics allows one to derive hysteresis cycles, and their dependence on temperature starting with only two parameters: the dielectric constant of the material and the maximum value of the dipole moment of a unit cell. Values obtained for Curie temperatures and coercive fields agree well with experiments. "Exact" energy dependencies on the asymmetry parameter are derived, and their connection with the Landau-Ginsburg-Devonshire is proven. By considering also the dipolar interaction in a continuous model, in addition to the ordering energy in presence of surface charge accumulation, one may estimate the distribution of the polarization inside the film and the validity of the hypothesis of uniform polarization. The above model was extended by considering that an essential parameter of this interaction is the permittivity of the film, assumed to be a material constant, together with the maximum value of an elemental dipole and the density of the elemental dipoles. These can be connected to three experimental parameters: the saturation polarization, the coercive field at zero temperature and the Curie temperature. For a ferroelectric material both the global and the differential permittivity depend on the temperature and on the polarization. This raises the question whether such a non-constant permittivity should be used in the stabilization energy of the ferroelectric phase, and whether it can be identified self-consistently with the function resulting after applying the statistics based on the microscopic model. In such case, a mutual interdependence should exist between the above three parameters. A model is built up, however the coercive field and the Curie temperature yield values several orders of magnitude higher than the experimental ones. Therefore, one has to introduce a background dielectric constant to accommodate the result of the model with the experimental data. The poling history of the film has to be taken into account, together with the presence of a small bias field. The model is able to predict self-consistently the equation of state of a ferroelectric, and in particular the linear decrease of the coercive field with temperature. The microscopic parameters, in particular the background dielectric constant and the density of elemental dipoles may be expressed directly from experimental quantities [2].

References:

[1] C.M. Teodorescu, Phys. Chem. Chem. Phys. 23 (2021) 4085–4093.
[2] C.M. Teodorescu, Phys. Chem. Chem. Phys. 24 (2022) 5419–5430.

NOTES

ORAL PRESENTATION

S2-OP8

Investigating the chemical and structural evolution of sub-monolayer Sn on Au(111)

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In this study, we investigate the influence of layer thickness on the structural and chemical characteristics of sub-monolayer Sn phases atop the Au(111) surface, focusing in particular on structural phases with less than 1/3ML Sn film thickness. Stanene, the two-dimensional hexagonal arrangement of tin, is predicted to have similarly exceptional electronic properties as graphene. In addition, due to its heavier mass and increased structural buckling, stanene is predicted to exhibit topological properties even at RT, making it a compelling candidate for future two-dimensional topological devices [1]. As the surface and interface structure of low-dimensional materials are known to be key determinants of their electronic properties, our analysis focuses on the surface and interface structure of the sub-monolayer Sn phases obtained for coverages of less than 1/3ML of Sn film thickness on Au(111).

Here, we report on the structural and chemical investigation of different sub-monolayer Sn phases on Au(111) using low-energy electron diffraction (LEED), scanning tunneling microscopy (STM), photoelectron spectroscopy (XPS), and photoelectron diffraction (XPD). Gradually, tin layers of different thicknesses between 1/4ML and 1/3ML were deposited on the Au(111) surface by physical vapor deposition. Our results reveal that subtle variations in Sn film thickness exert significant effects on the arrangement of Sn atoms atop the Au surface. Notably, we observed two distinct hexagonal arrangements of Sn with only minor differences in film thickness. At a film thickness of 1/4ML, we observed a 2x2 reconstruction, and at a thickness of 1/3ML, a stripe-like phase emerged, reminiscent of the herringbone reconstruction observed on the clean Au(111) surface. Our XPD analysis confirms this phase to possess an unusually large unit cell reconstruction of sqrt(3)x27. Further investigations at higher Sn coverages revealed that this stripe-like phase serves as a template for the diverse structural phases observed at coverages of approximately 2/3ML Sn on Au(111).

Our findings therefore contribute to a deeper understanding of the interfacial structure of Sn on Au(111), and especially the investigation of the stripe-like template phase provides valuable insights for the preparation of freestanding stanene. Our investigations tie in with our recently published results of the investigation of germanene on Ag(111)[2].

References:

[1] A. Molle, J. Goldberger, M. Houssa, et al., Nature Mater. 16 (2017) 163–169.
[2] L. Kesper, J.A. Hochhaus, C. Westphal, et al., Sci. Rep. 12 (2022) 7559.

NOTES

ORAL PRESENTATION

S2-OP9

Chemical vapor deposition of octadecyltrichlorosilane monolayer films on plasma-activated silicon substrate

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Deposition of octadecyltrichlorosilane (OTS) layers is commonly used in electronic industry for fabrication of thin dielectric films [1] and in micro- and nano-technology applications that require functionalization of silicon surfaces to obtain low friction, wearing resistant, anti striction and low surface energy [2]. Usually, OTS monolayer films are obtained on silicon or silica based on wet chemistry techniques comprising self-assembled monolayers (SAMs) deposition of OTS from solutions on surfaces that were previously activated by piranha solution. However, this technique does not allow for a good control of the process, which depends on solvent purity, humidity of the environmental air, and thus may yield inhomogeneous depositions [3]. Particularly, presence of the water in solvents or in air play an important role since it has been proved that OTS molecules do not bond directly to hydroxylated silica surface and presence of a molecular film of water adsorbed on surface is required [4].

In this work we use low-pressure plasma of a luminescent discharge in air and water vapor to activate (clean and hydroxylate) silicon surface followed by chemical vapor deposition of OTS on the plasma-activated surfaces. Between the two fabrication steps we add an additional step consisting in exposure of the activated silicon surface to water vapor at relatively low pressure (8 mTorr). The whole fabrication process is realized in the same deposition chamber at low pressure, thus preventing surface contamination. Results showed that the second step of the fabrication process is extremely important, since adsorption of too much water on the hydroxylated silicon surface leads to formation of particulate aggregates of OTS, while insufficient adsorption of water results in formation of sub-covered OTS surfaces.

References:

[1] M. Devynck, et al., Eur. Phys. J.: Appl. Phys. 56 (2011) 34106.
[2] S. Watson, et al., RSC Adv. 5 (2015) 89698.
[3] M. Hancer, Progr. Org. Coatings (2008) 63, 395–398.
[4] P. Silberzan, et al., Langmuir 7 (1991) 1647.

NOTES

ORAL PRESENTATION

S2-OP10

Thin films characterized by the precession of the electron beam

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The precession system for electron diffraction is an electronic system that on coils in the microscope column to perform the operations of rotating the electron beam. The rotation of the fascicle is done with the help of an alternative signal applied to the deflections coils terminals (used to tilt the fascicle in normal working mode), respectively to the DESCAN coil terminals, to refocus the fascicle in the direction of the optical axis.

Electron diffraction is an additional technique in electronic microscopy studies. Since the XRD or neutron diffraction techniques was used intensely for crystalline structure determination, electron diffraction has potential for special cases were even this technique fails. Due to several factor the electron diffraction is not suitable for crystal structure determination, but with hardware and software improvement we can transform this technique in useful one.

We show here an example of analysis of some different samples using combined technique, such as TEM/HRTEM image, electron diffraction without and with improvement provided by a precession system. We highlight the cases were electron diffraction succeed and the cases were failed, even the precession system is used.

To highlight the improvement of the results obtain by using the applied precession system electron diffraction (PED) we performed a study on a series of some samples, having different compositions and crystal structures.

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ORAL PRESENTATION

S2-OP11

New insight into the angular distribution of multi-elemental oxide thin films grown by pulsed electron beam deposition

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The control of stoichiometry is of critical importance to attain the desired functional properties in metal oxide thin films for applications, regardless of the thin film growth method. In the case of multi-elemental oxide thin films like barium strontium titanate $Ba_xSr_{1-x}TiO_3$ (BST), the electric and dielectric properties of thin films are strongly depending on the composition [1]. We developed the pulsed electron beam deposition method (PED) as an alternative to the pulsed laser deposition method (PLD), using the ablation plasma for the growth of thin films with complex compositions and tunable physical properties. PED is typically used to grow oxide thin films on planar substrates (10 mm x 10 mm) and only few papers have studied the angular dependence of ablation plasma species on large area substrates in PLD [2] and PED [3].

We present measurements of the angular thickness and composition profiles of thin films up to 90° obtained by irradiating a BST (x=0.2) target with the pulsed electron beam. A semi-sphere holder was used with a fixed 40 mm target to substrate distance at all angles [2, 3]. These large area BST thin films, grown by PED either in argon or oxygen background gases at a pressure of about 10^{-2} mbar and room temperature, were analyzed by Rutherford backscattering spectrometry (RBS) at different angular positions. The film thickness profiles present forward shaped peaks, with measurable thickness up to 80-90° for the major axis and up to 25° for minor axis, presenting similar trend for both argon and oxygen background gas. The analysis of the congruent transfer of the elements from the target as function of the angle showed that the film composition is not uniform over this large angular range, depending on the mass of the target elements, background gas and fluence. Complementary X-ray photoelectron spectroscopy was performed on large area BST thin films and compared with RBS measurements, revealing a stronger variation of stoichiometry at the surface compared to the bulk of the films.

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References:
[1] J.P. Goud, et al., Adv. Electron. Mater. 7 (2021) 2000905.
[2] A. Ojeda, et al., Appl. Surf. Sci. 336 (2015) 150–156.
[3] D. Dobrin, et al., Appl. Surf. Sci. 657 (2024) 159757.

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ORAL PRESENTATION

S2-OP12

Tailoring perovskite-based thin films to boost photoelectrochemical water splitting efficiency

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Photocatalysis represents a promising avenue for addressing two pressing global challenges: the need for sustainable energy generation and the mitigation of environmental pollution. One of its key advantages lies in its ability to harness the limitless energy provided by sunlight. Within this field, perovskite materials have emerged as particularly exciting candidates for photocatalyzing various reactions, including the process of water splitting, which represents an immense potential for renewable energy production. To maximize the efficiency of perovskite-based photocatalysts, a detailed study of their structure and composition is essential. This involves fine-tuning their inherent properties, such as crystal structure, surface morphology, and chemical composition, to optimize their performance in photoelectrochemical (PEC) processes. Precisely adjusting these characteristics enhances the materials` ability to absorb light, facilitate charge separation, and catalyze desired reactions with high efficiency. In our study, we focus on the fabrication of perovskite thin films using Pulsed Laser Deposition (PLD), which allows for precise control over film thickness and deposition conditions. By systematically varying these parameters, we investigate their impact on the performance of the resulting photoelectrodes in PEC applications. Specifically, we explore changes in film thickness and oxygen content and their influence on the structural and photoelectrochemical properties of epitaxial $LaFeO_3$ (LFO) thin films. We analyze the behavior of these perovskite-based photoelectrodes through potentiodynamic and potentiostatic PEC measurements in a strong alkaline solution. Utilizing advanced characterization techniques such as X-ray diffraction, high-resolution transmission electron microscopy, and ellipsometry, we gain insights into the correlation between the structural, topographical, and optical properties of the materials and their photocatalytic performance. Our findings reveal that the thinnest LFO/Nb:$SrTiO_3$ sample, prepared under specific deposition conditions, exhibits the highest photocurrent density values and remarkable stability over time. This highlights the importance of precise control over material synthesis parameters in achieving superior PEC performance. Further enhancement in photocurrent density is expected through the use of a multilayer photoelectrode incorporating LFO and BFO materials. Importantly, perovskite-based thin films exhibit efficient hydrogen evolution from water, confirmed by gas chromatography under constant illumination. The enhancement of photocurrent density can be achieved through the utilization of a multilayer photoelectrode incorporating LFO and BFO materials. The objective of this investigation was to merge the robust ferroelectricity of BFO with the excellent absorption properties and high chemical stability of LFO, thereby creating novel photocatalysts with improved activity in photocatalytic reactions.

NOTES

ORAL PRESENTATION

S2-OP13

Hierarchical nanostructure for energy and sensing application

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Developing facile methods for the synthesis of thin films and active and stable hierarchical nanostructures is of great interest. It consists of higher assembly-level of constituents by low dimensional nano-building blocks which has received an extensive attention in the latest advancements in nanomaterial science and nanotechnology development. The ordered hierarchical nanostructures could offer merits such as more active sites, synergistic properties owing to their geometric complexity and building blocks variation, as well as the resultant multi-functional capabilities. Indeed, obtaining materials of controlled size and shape at the nanometric scale is a necessary prerequisite to develop many applications.

We are therefore interested in optimizing the physical methods combined with drift approaches soft chemistry synthesis techniques like mist CVD, spray pyrolysis, SILAR, electrodeposition, and hydrothermal to grow high quality thin films layers and stable hierarchical nanostructures.

In this presentation we will focus on the preparation of thin films based ZnO, ZnS, CZTS, nanowires and dendritic silver nanoparticles. We will also present some application of such nanostructures

References:

[1] I. Jellal, et al., Opt. Quantum Electron. 55 (2023) 620.
[2] Y. Khaaissa, et al., Materials Today: Proc. 290 (2022) 126481.
[3] M.Y. Zaki, et al., Opt. Mater. 83 (2018) 252–256.
[4] K. Nouneh, et al., Int. J. Nanoscience 20 (2021) 2150056.
[5] P. Prieto, et al., App. Surf. Sci. 258 (2012) 8807–8813.
[6] A. Taleb, et al., Nanotechnol. 22 (2011) 205301.

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ORAL PRESENTATION

S2-OP14

Advanced synthesis techniques of 2D materials for enhanced functional properties

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Two-dimensional (2D) materials have emerged as foundational elements in the development of advanced technologies due to their unique properties, such as high electrical conductivity, transparency, flexibility, and high surface area. The effectiveness of these materials, particularly in innovative electronic and energy storage applications, depends on the synthesis methods employed, which directly influence their physical, chemical, and functional properties. This work explores various innovative synthesis techniques of 2D materials such as CrSe, SnSe, WS_2, and MoS_2, highlighting the impact of these methods on the materials capabilities in applications ranging from cryogenic temperature sensing to memristive devices. Our approaches, including physical vapor deposition followed by and space-confined sulfurization, chemical vapor deposition and liquid exfoliation are tailored to enhance specific desirable properties. Notably, micrometer-sized hexagonal CrSe flakes exhibit superior sensitivity in cryogenic temperature applications. Similarly, layered SnSe and MoS2 thin films, synthesized by eco-friendly processes, demonstrate enhanced phonon properties and memristive characteristics suitable for low-power computing. The production of horizontally aligned MoS_2 nanosheets via a unique CVD method results in an increased abundance of catalytic sites, promising for energy conversion technologies. Additionally, the synthesis of WS_2 ultrathin films and direct GrapheneMoS_2 heterostructures underpins the versatility of 2D materials in next-generation applications. This work not only advances our understanding of 2D material properties depending on the synthesis method but also significantly broadens their scope in technological applications.

NOTES

ORAL PRESENTATION

S2-OP15

Preparation of $CuSn_2S_3$ (CTS) thin films through sulfurization of electrodeposited Cu-Sn stacked precursor layers

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Cu_2SnS_3 (CTS) thin films were fabricated via the sulfurization process of electrodeposited Cu-Sn precursor stacks on Mo-coated glass substrates. The metallic layers were deposited at various Sn deposition potentials (-0.9 V, -1.05 V, and -1.2 V) and subsequently sulfurized under Argon atmosphere conditions at 450 °C for 10 minutes to yield CTS films. Through analysis using Raman spectroscopy and X-ray diffraction, it was observed that all stacked depositions at different Sn deposition potentials exhibited a single tetragonal CTS phase with excellent crystallinity and a prominent 112 peak. Scanning electron microscopy (SEM) images revealed a compact, homogeneous morphology with densely packed grains in the CTS films. Notably, the film deposited at -1.2 V of Sn demonstrated superior homogeneity. Energy-dispersive X-ray spectroscopy (EDAX) spectra of the sulfurized alloy precursors confirmed the formation of CTS. This study presents novel insights into the electrodeposition of CTS thin films via stacked precursors, offering potential applications in device fabrication.

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ORAL PRESENTATION

S2-OP16

The morphostructural and optical characteristics of SnO_2 films deposited by picosecond laser ablation

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SnO_2 films starting from metallic Sn target in oxygen atmosphere at several pressures, 150, 300, 450 and 900 mTorr were deposited using a picosecond Nd:YVO4 laser (355 nm/ 50 kHz, 0.25 W). After deposition at room temperature (RT) / FTO (fluorine doped tin oxide) substrate, the films were annealed in oxygen atmosphere at 350/450/550 °C. The films were investigated from structural, morphological, (surface and cross section) thickness, porosity and optical point of view. The influence of the experimental deposition parameters on the films characteristics was studied. The films were completely oxidized after annealing at 550 °C in oxygen atmosphere and presented high porosity with oxygen pressure increasing. The size of the particles was in the range of 37 – 480 nm and decreased with thermal annealing of the films. At RT, the film thickness was in the range of 2.03 – 3.42 µm while at 550 °C, it was in the range of 1.10 – 1.57 µm. The best film transmission was obtained for the films annealed at 550 °C and at 150 mTorr oxygen pressure.

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ORAL PRESENTATION

S2-OP17

Emerging properties in ferromagnetic semiconductors through interfacial charge-spin transfer in nanocomposites with half–metals

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To create ferromagnetically ordered semiconductors, especially with intrinsic defects and/or spin-polarized doping, we utilize charge and spin transfer across interfaces in composite nanomaterials with ferromagnetic elements. At the interfaces between semiconductors and half-metals (HM), only spin-polarized states related to or from the Fermi level (FL) of the HM are relevant. These materials are typically nanostructured, either in layered or particulate forms. Spin polarization and ferromagnetic ordering in the semiconductor can occur via a spin injection current or through spin diffusion, where charge/spin carriers spontaneously diffuse (wave function tunneling), inducing ferromagnetic order, typically in the presence of various defects as vacancies or spin polarized states resulted from doping. Interface charge/spin transfer can exploit some spin-orbit coupling effects, with band alignment being crucial for facilitating efficient charge and spin transfer across the heterostructure interface. These nanocomposites exhibit combined ferromagnetic, semiconducting, and other functional properties, enabling their use in various applications or their integration into versatile devices with novel magnetic, electronic, and optical functionalities.

In our study, we synthesized thin films and nanoparticles of various half-metals, subsequently coating them with wide bandgap semiconductors. Cobalt ferrite, magnetite, and Fe_50Pt_{50} (L10) alloy nanoparticles were paired with TiO_2, ZnO, ZnS, or SnO_2 semiconductors using chemical synthesis. FePt (L10) half-metal thin films were coated with ZnS or MoS_2 thin layers via pulsed laser deposition (PLD). Regardless of morphology, all composite systems exhibited ferromagnetic behavior in the semiconductors, facilitated by polarized charge-spin transfer at the interfaces, governed by energy band alignment. Sample characterization involved techniques such as X-ray diffraction, photoelectron spectroscopy, and electron microscopy to determine structure, composition, and morphology. Magnetometry, transport measurements, and optical absorption spectroscopy were employed to assess specific properties, with a focus on understanding interface charge/spin dynamics. Notably, in thin film materials, the competition between the RKKY and Rashba effects significantly influences ferromagnetic order within the semiconductors. Additionally, ferromagnetically ordered vacancies or impurities align antiparallel to the polarization source and, along with a minor yet significant Zeeman splitting, enhances the light absorption within the semiconductor, particularly in the sub-gap region (visible). The process, through local lattice relaxation, is assisted by phonons.

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ORAL PRESENTATION

S2-OP18

Study on the synthesis of gold/silver stabilized magnetite nanoparticles

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In our investigation, magnetite nanoparticles were produced using an adapted chemical co-precipitation technique [1], stabilized in aqueous dispersion with glucose, and coated with gold or silver [2,3]. We examined their microstructural characteristics of the core-shell nanosystems using Scanning Electron Microscopy, Transmission Electron Microscopy, and X-ray Diffraction, as well as their magnetic properties using Vibrating Sample Magnetometry. Dark field microscopy and UV-Vis spectrophotometry were utilized to examine the plasmonic properties based on the presence of a noble metal shell.

To evidence the impact on the environment following biomedical use, we conducted nanotoxicity studies on young vegetation photosynthesis, specifically on Cucumis melo seedlings, which have larger phloem vessels that facilitate nanoparticle circulation.

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ORAL PRESENTATION

S2-OP19

A portable and accurate fiber optic plasmonic sensor for environmental water pollutants monitoring

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These days, there are excessive amounts of heavy metals and persistent organic pollutants in the water environment, which causes pollution and poses major risks to public health [1]. Such environmentally dangerous compounds were detected using a variety of analytical techniques, such as electrochemistry, fluorescence, chromatography, mass spectrometry, or atomic absorption spectrometry.

Among them, the fibre optic-surface plasmon resonance (FO-SPR) method is particularly noteworthy since it offers quick, sensitive, real-time, label-free measurements with low sample consumption [2]. As a result, FO-SPR sensors have been used to evaluate water contamination and assess the water treatment procedure. With the right surface modification, the FO-SPR sensing system can identify the majority of environmental water contaminants [3].

The manufacturing and characterization findings of such FO-SPR sensors were disclosed in this work. Additionally, we employed these sensors to quickly and accurately identify pesticides (4-nitrophenol) [4] and heavy metals (cobalt, cadmium, zinc, and copper) [5] in water samples. For the later application, several plasmonic materials (gold, platinum, palladium) and polymers (polyaniline, chitosan, etc.) specific to the aforementioned heavy metals were sequentially coated on the FO-SPR sensor. Moreover, the FO-SPR sensor coated with a polyaniline/platinum bilayer and used for 4-nitrophenol detection, demonstrated a sensor limit of detection in the low pM concentrations range.

The FO-SPR sensors are amongst the most versatile tools, and their use might be extended to almost all types of pollutants present in water.

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References:

[1] S. Boruah, R. Biswas, Opt. Fiber Technol. 46 (2018) 152–156.
[2] A.K. Shakya, S. Singh, Opt. Laser Technol. 153 (2022) 108246.
[3] I. Antohe, Rom. Rep. Phys. 74 (2022) 505.
[4] I. Antohe, et al., Sci Rep 11 (2021) 10086.
[5] B.G. Solomonea, et al., Biosensors 12 (2022) 573.

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ORAL PRESENTATION

S2-OP20

Conductive polymers as chemiresistive ammonia gas sensing materials

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The importance of gas detection is undeniable for many industries including the healthcare industry and the environmental monitoring. The quick and precise detection of various gases such as ammonia (NH3) ensures not only workplace safety but also recognition of potential hazards and the management of emissions [1].

Taking into account all of the previously mentioned factors, the investigation of chemiresistive sensors based on conductive polymers (i.e. polyaniline, polypyrrole, etc) resulted from the need for sensors with high sensitivity, adaptability, and fast reaction times. With their ability to function at room temperature and the ongoing advancement of studies involving them, these sensors have become highly promising tools for gas detection [2].

For the present study, two conductive polymers, namely polyaniline (PANi) and polypyrrole (PPy), were chosen due to their noteworthy response in contact with NH_3 gas [3, 4]. Their synthesis was made through chemical polymerization of their monomer onto the interdigitated gold electrodes. Further characterization involved scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS), methods that offered insights about the sensors' morphological and chemical particularities. The electrical characterization of the fabricated sensors was performed using an in-house gas testing set-up and their electrical properties were investigated with a source-meter while the sensors were placed in the gas chamber and directly exposed to different concentrations of the analyte, ranging from 1 to 100 ppm.

Lastly, the data analysis demonstrated that the proposed sensors show steady response over time, good analyte sensitivity and selectivity. Response time was calculated as the time taken to reach 90% of the final resistance in the presence and absence of the target gas, respectively. The limit of detection (LOD) for both types of sensors was found to be below 1 ppm.

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References:
[1] M.A. Farea, et al., Chemical Physics Letters 776 (2021) 138703.
[2] L. Xianghong, et. al., Coordination Chemistry Reviews 462 (2022) 214517.
[3] M. Das, S. Roy, Materials Science in Semiconductor Processing 121 (2021) 105332.
[4] V. Gupta, Materials Chemistry and Physics 310 (2023)128388.

NOTES

ORAL PRESENTATION

S2-OP21

Atomistic approach to the strain field in finite-sized heterostructures

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The numerical code AS-LBFG-v2 developed to simulate the atomic elastic relaxation in finite-sized heterostructures is introduced. To minimize the elastic energy, the L-BFGS algorithm is utilized. A user-defined initial atomic configuration, without restrictions on the shape of the matrix embedding quantum dot (QD), can be implemented in the code. By enlarging the pyramidal QD heterostructure towards mesoscopic size, the code generates a strain field distribution similar to that obtained by continuum model for weakly polar semiconductors. The strain field obtained for semi-torus, and spherical shape QDs embedded in finite-sized matrices is also presented. The dependence of the strain field on the cap thickness and the distribution of misfit dislocations in the relaxed configuration are simulated by the code.

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The code is published on the Code Ocean platform of Comp. Phys. Comm. at: AS-LBFG-v2.
Atomistic approach of strain field in quantum dots: Structure relaxation. | Code Ocean

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ORAL PRESENTATION

S2-OP22

Single qubit control in the presence of other qubits

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Precise qubit control is paramount in all implementations of quantum computers. Various schemes, both adiabatic or non-adiabatic have been devised to implement high fidelity quantum gates for quantum processors, in order to mitigate the effect of noise, cross-talk between channels, stray fields, etc. Here we create a minimal model taking into account all relevant effects to the control of a superconducting qubit system. We model the control loop which implements the single qubit quantum gate on a qubit and estimate the gate fidelity under the effect of various decoherence mechanisms and the presence of other qubits.
In material manufacturing it is usually impossible to discriminate between the role and weight of each factor that may affect the structure composition at nanoscopic scale. This gap can be filled by computational modeling techniques and methods.

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ORAL PRESENTATION

S2-OP23

Computational tools in material science

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In material manufacturing it is usually impossible to discriminate between the role and weight of each factor that may affect the structure composition at nanoscopic scale. This gap can be filled by computational modeling techniques and methods.

One of the main directions of research within our group is the computational evaluation of material properties by using numerical models and methods from Density functional theory to molecular dynamics, which provide detailed information on the effect of substitutional disorder, defects, vacancies, pressure or temperature onto the manufacturing process.

In the past few years, we focused on three applications of computational analysis in material science: (i) support experimentalist scientists into developing new materials for batteries, (ii) the study of materials dedicated to quantum technologies - in particular the fabrication of superconducting qubits and (iii) the computational assessment of molecule-metallic surfaces interactions.

We will present here our results on calculated properties of aluminum oxide structures based on both DFT and molecular dynamics. The experiments are performed by our collaborators from QuCos Quantera project.

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References:

[1] D. Willsch, et al., Nat. Phys. (in press, 2024). https://doi.org/10.1038/s41567-024-02491-3.
[2] F. Valenti, et al., Phys. Rev. B 109 (2024) 054503.

ORAL PRESENTATION

S2-OP24

Fine-tuning fluxonium qubit devices for enhanced performance

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Superconducting circuits offer a promising path for creating qubits because they allow for easy adjustment of their underlying physics. We can enhance superconducting qubits through techniques like refining materials and optimizing circuit parameters. Our study focuses on devices built using the fluxonium qubit architecture. We`re investigating how these devices interact with their surroundings when connected to a readout resonator. By simulating fluxonium devices connected to resonators, we aim to understand how factors like anharmonicity, dispersive shifts, and decoherence rates are influenced by the physical properties of the circuit components. This research helps us grasp the behavior of fluxonium qubits better, which is essential for improving their performance in practical quantum computing applications.

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ORAL PRESENTATION

S3-OP1

Strain analysis in vanadium oxide thin films by Rietveld refinement

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Vanadium oxides (VO_x) compounds have unique properties that can be further exploited for a wide range of applications, such as charge storage, photodetectors, sensors, smart windows, thermochromic coatings or photocatalysis [1]. For example, vanadium dioxide (VO_2) reveals a significant change in the resistance (for microbolometers) or in the transmission spectrum (for thermochromic coatings) with changing temperature. On the other hand, the layered crystal structure of vanadium pentoxide (V_2O_5) leads to the reversible lithium-ion insertion/extraction processes, becoming suitable for electrochromic coatings and charge storage devices. It was showed that crystallite size and defects are strongly linked with the characteristics of the MIT (metal-insulator transition) in VO_2 [2], while higher texture coefficients on (001) in V_2O_5 could enhance the coloration efficiency in the range of -1 to +1 V, as well as the Li-diffusion in charge storage devices [3,4]. It is clear that a deep understanding of the crystal structure of the VO_x materials is required for developing new applications with enhanced physicochemical properties.

In this presentation, thin films of VO_2 and V_2O_5 were obtained by pulsed laser deposition (PLD) and spray pyrolysis technique (SPT) in different conditions. The microstructure of the prepared films was assessed non-destructively using X-ray diffraction in the framework of Rietveld refinement, which enables the calculation of the unit cell parameters, mean crystallite size and lattice strain. Other investigation tools, such as diffuse reflectance spectroscopy (DRS) or Raman spectroscopy support the Rietveld data. According to the experimental findings, the dislocations formed at the grain boundaries are further responsible for the transition from insulator to metallic phase, as well as for the electrochromic and charge storage ability of the material.

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References:

[1] P. Hu, et al., Chem. Rev. 123 (2023) 4353–4415.
[2] S.A. Bukhari, et al., Appl. Surf. Sci. 529 (2020) 146995.
[3] C. Romanitan, et al., Phys. Status Sol. (a) 219 (2022) 2100431.
[4] K. Mouratis, et al., Nanomaterials 10 (2020) 2397.

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ORAL PRESENTATION

S3-OP2

X-ray diffraction study of threading dislocations in epitaxial gallium nitride thin films grown by molecular beam epitaxy

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For decades, gallium nitride (GaN) has proven interesting to material scientists due to its physical properties that recommend it for a large variety of semiconductor devices applications. However, the presence of defects known as threading dislocations within its crystalline lattice can hamper its usability in different applications and thus the present work focused on finding a reliable means of experimentally determining their type and concentration within different GaN samples. In the Targets Laboratory of the Extreme Light Infrastructure – Nuclear Physics (ELI-NP) Institute, we have studied GaN thin films prepared by Molecular Beam Epitaxy (MBE) on Si (111), Al_2O_3 (0001), and 3C-SiC (111) substrates d covered with an AlN layer. X-ray Diffraction (XRD) was used to obtain the diffraction profiles of every sample in skew geometry with a Rigaku SmartLab system. Rocking curve spectra (ω scans) were obtained on both asymmetric and symmetric (hkl) planes in order to determine the density and correlation length of edge and screw threading dislocations, respectively, using a theoretical model developed by Kaganer et al. [1]. Our results show that depositing GaN on 3C-SiC (111) favors the production of thin films with the best crystalline microstructure, as shown by having the lowest measured dislocation density of $1.47 \cdot 10^{10}$ cm^{-2} and the highest correlation length and mean distance between two defects (dislocations).

References:

[1] V. M. Kaganer, et al., Physical Review B 72 (2005) 045423.
[2] V. L. Ene, et al., Materials 12 (2019) 4205.
[3] V. L. Ene et al., Nanomaterials 10 (2020) 197.
[4] A.B. Serban, et al., Nanomaterials 11 (2021) 1299.

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ORAL PRESENTATION

S3-OP3

NAP-XPS instrumentation and applications

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Over the last decades it has been possible to develop XPS systems that can work far beyond the standard conditions of high or ultrahigh vacuum. Thus, Near Ambient Pressure (NAP) - XPS has become a rapidly growing field and has demonstrated its capability in a wide variety of applications. Starting from operando studies of surface reactions in catalysis, the applications soon have been extended towards studies of processes at liquid/solid or liquid/gas interfaces. Nowadays, the NAP-XPS analysis technique has become a standard analysis tool not only at synchrotrons, but also in laboratories. The availability of different optimized sample environments (gases, liquids, electrochemical cells) as well as the combination of various analysis methods (NAP-SPM, IRRAS, NAP-HAXPES, etc.) allow for gaining insights into the fundamental processes that take place during a chemical reaction.

We present existing solutions for NAP-XPS analysis with an emphasis on SPECS latest developments of instruments and material analysis methods. Examples and results from existing NAP-XPS systems will be shown as well as future perspective of applications and scientific contributions of routine operando NAP-XPS.

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ORAL PRESENTATION

S3-OP4

Observing barium oxide on W(110) by low-energy, thermionic and photoemission electron microscopy

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The deposition of alkali earth metals on transition metals is of interest both in fundamental studies as well as for applications and is one of the classic problems in surface science [1]. These systems are used in electron emission devices or discharge lamps. The characteristics of such devices has been the subject of several studies. The details of the thermionic emission depends on the particular electronic structure of the alkali earth oxides and, in the ultrathin film regime, also on the transition metal used as substrate. A detailed characterization can be combined nowadays with ab-initio calculations which in turn suggest more efficient configurations for actual devices. A classic example is the deposition of barium and oxygen on a tungsten surface for use in thermionic emitters.

Following Kordesch and coworkers [2] we have turned to low-energy electron microscopy (LEEM [3]) to observe barium oxides growth. We have been recently growing barium oxide islands by high temperature molecular beam epitaxy under observation in low-energy electron microscopy, where changes in work function can be monitored by measuring the transition between mirror and diffraction imaging. By changing the growth conditions, we can modify the surface morphology. For example, growth at a temperature of 1000 K produces large, tens of micrometers wide, islands that partially cover the substrate. When the sample is heated above 870 K, strong electron emission is observed, allowing for the observation of the islands in ThEEM (Thermionic Electron Emission Microscopy). By tuning the growth we can thus change the distribution of islands on the surface, potentially allowing for "design cathodes" where the thermionic emission takes place from well-defined distribution of objects.

Acknowledgements:

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References:

[1] L.R. Koller, The Physics of Electron Tubes, MacGrawHill, New York (1937).
[2] J.M. Vaughn, et al., IEEE Transactions on Electron Devices 56 (2009) 794.
[3] Kevin F. McCarty, Juan de la Figuera, Low-energy electron microscopy, in: Surface Science Techniques, 51, 531 (2013) (Springer Berlin Heidelberg).

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ORAL PRESENTATION

S3-OP5

Surface magnetism of platinum (001) and strontium titanate (001) investigated by spin-resolved photoelectron spectroscopy

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This work presents results on the interplay between charge accumulation at surfaces and the occurrence of magnetism, investigated by direct measurement of spin asymmetry using spin-resolved photoelectron spectroscopy (SRPES). One way to assess such phenomena is to use the Stoner criterion [1]. Recently, a model was developed which takes into account the total one-electron energy in the spin-resolved sub-bands and not only the kinetic energy [2]. In a simplified way, systems where the derivative of the DOS at the Fermi level is negative will feature ferromagnetism. The (001) surface of metal platinum, featuring the hexagonal reconstruction [3] is a good candidate to test which model is the most valid. The Fermi level in bulk sits close to the maximum of the valence band, and the surface is electron enriched [4]. Therefore, one expects that the derivative of the DOS is negative at the Fermi level and according to [2] the spin asymmetry should manifest, whereas the Stoner criterion would not be fulfilled. This system was studied by scanning tunneling microscopy and low energy electron diffraction (LEED), featuring the hex reconstruction, then by core level photoelectron spectroscopy, certifying the negative chemical shift of the surface component, and SRPES, revealing a sizable spin asymmetry [5]. The second system which will be discussed is strontium titanate (001), investigated by LEED, core level photoelectron spectroscopy and SRPES, featuring a two-dimensional electron gas at the surface [6]. The most important part of the signal is exhibited by O 2p bands, which is interpreted as a signature of the indirect exchange interaction between these states intermediated by the surface two-dimensional electron gas [7].

References:

[1] E.C. Stoner, Proc. Roy. Soc. London 165 (1938) 372–414.
[2] C.M. Teodorescu, Res. Phys. 25 (2021) 104241.
[3] R. Hammer, et al., Phys. Rev. B 94 (2016) 195406.
[4] A. Baraldi, et al., J. Chem. Phys. 127 (2007) 164702.
[5] L.E. Borcan, et al., Appl. Surf. Sci. submitted (2024).
[6] A.F. Santander-Syro, et al., Nature 469 (2011) 189–193.
[7] J.M.D. Coey, et al., J. Phys. Condens. Matter 28 (2016) 485001.

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ORAL PRESENTATION

S3-OP6

The effects of ultrahigh vacuum treatments on SnSe flakes transferred on naturally oxidized Si wafers

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The as introduced samples, as well as the treated flakes were characterized by means of low energy electron microscopy (LEEM), LEEM I-V, survey in X-ray photoemission electron microscopy (XPEEM) at 100 eV for maximum surface sensitivity of the lines of interest O 1s, Sn 3d, Si 2p and Se 3d, X-ray photoemission spectroscopy (XPS) in dispersive mode at four different kinetic energies (630, 585, 200 and 155 eV) for maximum surface sensitivity for the photoemission lines mentioned before, as well as C 1s as valence band. We have also characterized the chemical states by near edge X-ray absorption fine structure (NEXAFS) at the Sn M, Se M and Si L edges. The samples did not show surface crystallinity as no low energy electron diffraction (LEED) patterns appeared, however the structures are 2D since a mild, 1 minute Ar+ sputtering treatment considerably reduced the thickness of the structures.

The flakes are highly affected by annealing and new interface phenomena occur during the solid state reaction at 350 °C in ultrahigh vacuum. In the XPS dispersive mode we see that Se replaces oxygen in the SiOx substrate, effect that is very clear in the Si 2p spectra and in O 1s. Se 3d signal decreases considerably showing that aside for the migration deeper into the substrate, some of it is also lost. After the annealing there is almost no Sn-Se present and most Sn interacts with O. Sn 3d and Se 3d spectra were acquired at the beginning of the 50 minutes annealing and also at the end of the treatment.

The measurements were performed at the Bessy II synchrotron, SMART beamline, in Berlin.

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ORAL PRESENTATION

S3-OP7

Intrinsic electronic structure of oxide surfaces and interfaces from angle resolved photoelectron spectroscopy

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Physics of the multiferroic interfaces is currently understood mostly within a phenomenological framework based on screening of the polarization field and depolarizing charges. Additional effects still unexplored are the band dependence of the interfacial charge modulation and the associated changes of the electron-phonon interaction, coupling the charge and lattice degrees of freedom. Here, multiferroic heterostructures of the colossal-magnetoresistance manganite $La_{1-x}Sr_xMnO_3$ buried under ferroelectric $BaTiO_3$ and $PbZr_xTi_{1-x}O_3$ are investigated using Soft-X-ray angle-resolved photoemission [1]. The experimental band dispersions from the buried La1-xSrxMnO3 identify coexisting two-dimensional hole and three-dimensional electron charge carriers. The ferroelectric polarization modulates their charge density, affecting the coupling of the 2D holes and 3D electrons with the lattice which forms large Fröhlich polarons inherently reducing mobility of the charge carriers. Moreover, we separate the band structure signature of the top FE layer from that of the bottom electrode. Despite intense studies of PZT over decades, its intrinsic band structure, electron energy depending on 3D momentum k, remained still unknown. Hence, the band structure of $Pb(Zr_{0.2}Ti_{0.8})O_3$ is obtained [2]. The enhanced photoelectron escape depth in this photon energy range allows sharp intrinsic definition of the out-of-plane momentum k and thereby of the full 3D band structure. Furthermore, the problem of sample charging due to the inherently insulating nature of PZT is solved by using thin-film PZT samples, where a thickness-induced self-doping results in their heavy doping. For the first time, the soft-X-ray ARPES experiments deliver the intrinsic 3D band structure of PZT as well as the FE-polarization dependent electrostatic potential profile across the PZT film deposited on $SrTiO_3$ and $La_xSr_{1-x}MnO_3$ substrates.

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References:

[1] M. A. Husanu, et al., Communications Physics 5 (2022) 209.
[2] D. G. Popescu, et al., Advanced Science 10 (2023) 2205476.

NOTES

ORAL PRESENTATION

S3-OP8

Advanced method for amino acid recognition within peptide sequences

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The development of methods and strategies to identify and accurately quantify amino acids sequences in single peptides and proteins is a prominent and expanding field [1,2]. Single-molecule sequencing of peptides by direct, real-space imaging that would have the potential to identify composition, structure, conformation and properties of peptides and peptide-related compounds would open new avenues in omics-research [3].

Established sequencing routes at the single molecule level rely on fluorescent labelling using markers, employ tunneling current measurements between metallic electrodes, or measurements in nanopores functionalised with recognition molecules. Single molecule imaging techniques that provide structural information resolved at the sub-nanometer scale can directly access local conformations and inter- and intramolecular bonding. However, local readout of chemical information is not available.

In this work, we introduce a probe-sensitisation procedure to reliably determine the location of one specific amino acid within different peptide sequences using a low temperature scanning tunneling microscopy (STM) [4]. The mechanism is based on a selective intermolecular interaction between a sensitiser molecule attached at the apex of the STM tip and the target amino-acid on the surface incorporated in the peptide. The amino acid specific interaction induces an enhanced tunneling conductance of one spectral feature mapped in spectroscopic imaging and then associated to the location of one specific amino acid in the topography image. Density functional theory calculations suggest that the origin of the chemically specific interaction between the probe sensitiser and the amino acid within the peptide can be understood via a docking mechanism that modifies the geometry as well as local charge distribution of the molecular probe. The proof-of-concept of this procedure is demonstrated for the amino acid tryptophan in several different peptide sequences, that are deposited intact on a clean surface in ultrahigh vacuum after mass selection by using an electrospray ion beam deposition technique. Thus, our study provides a new step towards single-molecule proteomics.

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References:

[1] V. Marx, Nat Methods 16 (2019) 809–812. [2] C. Seydel, Nat Methods 19 (2022) 1036–1040. [3] L. Restrepo-Pérez, et al., Nature Nanotech 13 (2018) 786–796. [4] X. Wu, B. Borca, et al. Nat Commun 14 (2023) 8335.

NOTES

ORAL PRESENTATION

S3-OP9

Momentum estimation of charged particles registered in a nuclear emulsion detector within the DsTau(NA65) experiment

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The DsTau(NA65) is an experiment at CERN-SPS approved by CERN in 2019, aiming to investigate tau neutrino production and to reduce the systematic uncertainty of its flux to 10%, only 9 events being directly registered in the DONuT experiment. A precise measurement of the tau neutrino cross-section would enable a search for new physics effects, such as testing the Lepton Universality (LU) of the Standard Model in the case of neutrino interactions. The main source of tau neutrinos is the sequential decay of the DS mesons produced in interactions of 400 GeV/c protons with a tungsten/molybdenum target: This decay has a peculiar "double kink" topology, where the kink angles and flight lengths are very small. Due to these characteristics, the only detector suitable to register this type of decay is the nuclear emulsion thanks to its excellent spatial resolution (50 nm). It is expected that around 1000 DS → tau + tau neutrino, tau → X + tau neutrino decays will result from the interaction of 2.3×10^8 protons with tungsten/molybdenum targets, along with the collection of 10^5 charm pairs.

This presentation will primarily focus on the momentum estimation of charged particles registered in the DsTau(NA65) nuclear emulsion detector using the Multiple Coulomb Scattering (MCS) method. MCS is a reliable technique used for estimating particle momenta by analyzing charged particle scattering in materials. This allows for precise momentum estimation by measuring the angle difference of a particle`s trajectory before and after interacting with tungsten/molybdenum plates.

During the 2023 DsTau(NA65) physics run, two special nuclear emulsion detection modules were developed to validate the momentum estimation method. These modules will undergo scanning at the Hyper Track Selector (HTS) microscope in Japan, followed by data analysis in the coming months.

NOTES

ORAL PRESENTATION

S3-OP10

Fabrication of a thin-film adaptive electrostatic phase plate

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Electron beams have become an integral technology for the fabrication and the characterization of micro and nanostructured devices. To further improve and advance this technology, control of the electron beam phase is one of the key elements that must be tackled. This work investigates the options in the fabrication process of electron phase plates (PP), considering the limitations imposed by 1) current cleanroom technology, 2) requirements for implementation in a transmission electron microscope (TEM), and 3) requirements for in-situ electric field adjustment.

The phase plate (PP) family consists of 5 different areas [1], with the two most investigated being thin-film based PPs [2] and electrostatic PPs [3]. Thin-film based PPs introduce the phase shift by a sharp phase cut-on, while electrostatic PPs instead introduce the phase shift through an electric field. This work combines the two concepts and investigates the possibility of fabricating a thin film membrane with electrodes on top, which has the combined benefits of hole-free and electrostatic PPs. This, however, introduces new limitations, as the membrane must be as thin as possible, while maintaining the stability to support the electrode system. In our design, the electron beam passes through a series of 6 concentric rings with different applied voltages. The values of the 6 applied voltages were simulated using COMSOL for obtaining the desired phase profile.

This PP design is intended for the condenser system of a typical TEM, where the beam size is ~50 µm. Consequently, we set the inner diameter of the outer grounded electrode at 50 µm. Furthermore, the PP is designed to interface with the Fusion select commercial holder, for which the relative beam positioning and electrode pads are well known. The membrane window itself will is etched as a square opening due to the crystal structure of silicon and fabricated such that the side length corresponds to double the beam diameter (100 µm). The fabrication process includes two critical steps: silicon etch and electrode fabrication. A compromise solution is to start with a partial KOH etch to thin the silicon to 25%, followed by electrode fabrication, and concluding with KOH etch of the remaining silicon.

With the fabrication completed, the next step is to properly test the PPs in the sample position in a TEM system and compare the obtained phase to simulation results. Here, the simulated phase profile will be compared with experimental results, where the phase will be mapped using Fresnel imaging.

References:

[1] M. Malac, et al., Microscopy 70 (2021) 75–115.
[2] K. Nagayama & R. Danev, Phil. Trans. R. Soc. B 363 (2008) 2153–2162.
[3] M. Malac, et al., Ultramicroscopy 108 (2008) 126–140.

NOTES

ORAL PRESENTATION

S3-OP11

PEM electrochemical hydrogen compressor evaluation

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Electrochemical hydrogen compression is a promising technology for compressing hydrogen gas efficiently and sustainably. It typically involves using proton exchange membrane (PEM) electrolysis cells operating in reverse mode to compress hydrogen by applying an electrical current. Compared to traditional mechanical compressors, electrochemical compression offers potential advantages such as lower energy consumption, quieter operation, and potentially lower maintenance requirements. In this paper we investigate the performance of a circular single-cell hydrogen electrochemical compressor with a 11.94 cm2 active area, using a Nafion 115 membrane at room temperature and 100 % RH. Pressure vs. time curves have been collected, and a pressure of 7 bar has been achieved with a single cell at an operating voltage of 0.030 V.

NOTES

ORAL PRESENTATION

S3-OP12

EPR investigation of the blue quartz from the Albesti - Romania granite

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Natural and synthetic quartz has been intensively studied over the years, using different investigative techniques, including electron paramagnetic resonance (EPR) [1]. Natural blue quartz is one of the least investigated varieties of quartz and, up to now, the color origin has not been clearly elucidated. There are over 500 areas in the world where blue quartz can be found, some of them being in Romania. The natural blue quartz from the Albesti granite (South Carpathians, Romania) loses its color at temperatures higher than 300 °C [2]. This work is focused on the investigation of the paramagnetic point defects in the Albesti blue quartz. EPR investigations in the X-band (9.5 GHz) and Q-band (34 GHz) were carried out on three colored – colorless pairs of quartz samples extracted from three different granite rocks, pristine and after isochronal annealing in the 100 – 500 °C range. The colored quartz samples were blue, pale blue, and milky white, respectively. In all our quartz samples we identified the paramagnetic Mn^{2+}, E`, and [AlO4]0 centers. The pale blue and its colorless partner quartz samples contained the largest amount of Mn^{2+} centers. In the milky white and their colorless counterpart quartz samples, broad EPR lines associated with magnetic clusters were observed. The isochronal annealing treatment up to 500 °C induced the recombination of the E' and [AlO4]0 centers, as reported before [3], the decrease of the Mn^{2+} spectrum, and the formation of a minority iron oxide phase. The EPR signatures of the matching colored and colorless natural quartz samples were similar before and after annealing, indicating that the heat-sensitive coloration of the Albesti natural quartz is not caused directly by the presence of paramagnetic defects and/or minority magnetic phases.

Acknowledgments:
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References:

[1] B.D. Perlson, J.A. Weil, Canadian Journal of Physics, 86 (2008) 871–881.
[2] A.I. Pantia, A.E. Filiuta, Carpathian Journal of Earth and Environmental Sciences, 16 (2021) 175–186.
[3] M.G. Jani, R.B. Bossoli, L.E. Halliburton, Phys. Rev. B. 27 (1983) 2285–2293.

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ORAL PRESENTATION

S3-OP13

Enabling Progress in Advanced Materials Research: Verder Scientific's Innovative Solutions

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The pursuit of breakthroughs in advanced materials research necessitates not only innovative methodologies but also the availability of cutting-edge scientific instrumentation. Verder Scientific, a key presence in the sphere of scientific instrumentation, introduces a comprehensive suite of advanced solutions, that have the potential to reshape the landscape of materials science research.

For decades, our manufacturing companies have been providing solutions for individual customer requirements by developing sophisticated, precise, and reliable laboratory equipment for sample preparation, heat treatment and analysis of solid materials. These solutions enable our customers to make progress. We provide them with the means to effectively and reliably design their processes, products, and services to become safer, more efficient, and more sustainable.

RETSCH is the leading solution provider for neutral-to-analysis sample preparation and characterization of solids. Based on a century of experience RETSCH develops size reduction and sieving equipment which is characterized by excellent performance, operating convenience, safety and a long lifetime. MICROTRAC MRB, a technology leader, committed to innovation, an unrivalled range of technologies for particle characterization. ELTRA is one of the world`s leading manufacturers of elemental analyzers for rapid and accurate analysis of solid materials. Our elemental analyzers provide tailor-made solutions for a wide range of samples and concentrations. Thousands of satisfied customers worldwide are proof of the quality and reliability of ELTRA analyzers. CARBOLITE GERO is a leading manufacturer of high temperature furnaces and ovens from 30 °C to 3000 °C with a focus on vacuum and special atmosphere technology. With more than 80 years of experience in thermal engineering our products are used in research laboratories, pilot plants and manufacturing sites worldwide.

In a research landscape increasingly dependent on instrumental capabilities, this presentation offers an opportunity to evaluate the role of Verder Scientific`s products as an enabler of scientific progress in the domain of advanced materials research.

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ORAL PRESENTATION

S3-OP14

Correlations between the synthesis route, morphology, structure and electrical properties of SnO_2-Gd_2O_3 nanocomposites for applications in gas sensing

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Semiconductor gas sensors based on metal oxides (MOX) are increasingly used for monitoring the concentration of toxic gases. However, despite their versatility and integration potential within complex semiconductor devices, detecting CO_2 using MOX gas sensors is quite challenging, because of the rather low reactivity of CO_2. Our study is focused on identifying the interaction mechanism between CO_2 target gas and SnO_2, Gd-doped SnO_2 and Gd_2O_3 sensing materials in the presence of humidity. For the correct assessment of the sensing response of these materials upon CO_2 exposure, it is important to understand also the role played by their morphology and structure, along with the fine electrochemical and charge transfer processes.

The samples were synthesized using co-precipitation (CP) and hydrothermal (HT) routes [1, 2]. To determine the morpho-structural properties, different analytical TEM techniques were employed: conventional TEM (CTEM) and high-resolution TEM (HRTEM) – to determine the morphology and the structure; selected area electron diffraction (SAED) – to identify the crystal structure; scanning TEM combined with energy-dispersive X-ray spectroscopy (STEM-EDS) – to determine the spatial distribution of the elements. These results were correlated with the structural information obtained from XRD and the sensor electrical response obtained from measurements performed under CO_2 and controlled humidity conditions. SnO_2 synthesized by co-precipitation was doped with different concentrations of Gd: 0.1%, 1%, 5%, 10% and 20%. The TEM investigations revealed some differences between the highly-doped and the weakly-doped samples, as SnO_2-Gd_2O_3 nanocomposites begin to form for high concentrations of Gd. Their presence was confirmed by SAED and also by CTEM and STEM-EDS. Pure Gd_2O_3 was also synthesized. The electrical measurements in controlled atmosphere have shown that the highest sensor response at 50% RH was for Gd_2O_3 [1].

For comparison, Gd_2O_3 was synthesized by hydrothermal route. Gd_2O_3-HT and Gd_2O_3-CP were also studied using the above-mentioned TEM techniques and the results revealed minor differences between the morphology and the structure of the two samples. On the other hand, the sensing measurements have shown that the sample Gd_2O_3-HT has a higher sensor response compared to Gd_2O_3-CP, at 50% RH [2].

Acknowledgments:

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References:

[1] C. Ghica, et al., Sens. Actuators B Chem. 368 (2022) 132130.
[2] C. E. Simion, et al., Mater. Chem. Phys. 296 (2023) 127354.

NOTES

ORAL PRESENTATION

S3-OP15

Fine-tuning of S/(S+Se) ratio in magnetron-sputtered CZTSSe thin films for improved characteristics

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The demand for kesterite $Cu_2ZnSn(S,Se)_4$ (CZTSSe) thin films in photovoltaic applications is significant due to their composition of environmentally friendly, earth-abundant elements and compatibility with established photovoltaic technologies. This study introduces a novel synthesis approach for CZTSSe films, varying the S/(S+Se) ratios from 0.83 to 0.43 through a dual-stage magnetron sputtering deposition/annealing process. The initial deposition produced stacked Mo-SnS_2-Cu layers, which, through sulfur-rich thermal treatment, transformed into Cu_2SnS_3 (CTS) films. Subsequent deposition of ZnSe and annealing in a tin and selenium atmosphere led to the formation of CZTSSe films. These processes were meticulously designed to fabricate high-quality, defect-reduced CZTSSe films, minimizing the occurrence of secondary phases and impurities. Characterization techniques, including grazing incidence X-ray diffraction and Raman spectroscopy, confirmed a compositional and structural transition from CZTS to a nearing CZTSe phase. Additionally, scanning electron microscopy revealed a correlation between decreased S/(S+Se) ratios and improved film densification and grain size. This study advances kesterite-based solar cell technology by enhancing the structural integrity and crystallinity of the absorber layer, essential for improving photovoltaic performance.

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ORAL PRESENTATION

S3-OP16

Facts and artifacts in optical and structural characterization of emerging materials for renewable and sustainable energy

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The p-type emerging materials for photovoltaics such as inorganic chalcogenides and organohalide perovskites or other materials for renewable and sustainable energy applications in thin film or powder form are often reported with misleading/wrong optical and structural parameters. Thus, the credibility and significance of many published works should be questioned by the readers. Following a smart documentation by note taking including mind mapping, any should create an integrated protocol to find out the truth.

First issue concerns the XRD analysis. Several pathways will be given to identify correctly the crystalline phase, the lattice parameters, to find out and to prove the existence or absence of secondary phases and to determine the average crystallite sizes.

Second problem regards optical measurements and methods to extract the band gap. Can at least qualitatively observe the band gap difference within a samples batch? Is considered the possible differences between surfaces of the films and their bulk? Examples on inorganic chalcogenides and on organohalide perovskites will be given.

Also, tips and tricks concerning complementary techniques such as Raman spectroscopy and X-ray photoelectron spectroscopy will be revealed, needed to sustain the conclusions or, why not, to change even the initial scientific findings.

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NOTES

ORAL PRESENTATION

S4-OP1

Strategies for achieving steady-state negative capacitance in ferroelectric multilayered structures

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Efforts to understand and regulate the switching dynamics and intricate electrostatic configurations of ferroelectric (FE) structures toward achieving negative capacitance (NC) regimes have intensified. This surge is driven by challenges in transistor scaling and enhancing energy efficiency. Proposed solutions explore augmenting gate oxide capacitance to minimize voltage drop. Despite the promise of high-k dielectrics, inherent limitations persist. Even with ultra-thin equivalent oxide thickness (EOT) SiO_2 gate oxides, a fundamental threshold of 60 mV/dec exists for substantially altering drain current. Salahuddin and Datta proposed NC in 2008 to transcend this barrier, suggesting negative oxide capacitance could overcome the Boltzmann limit, amplifying surface potential. Consequently, negative capacitance field-effect transistors (NCFETs) could circumvent both EOT and Boltzmann limits, enhancing energy efficiency.

Literature explores two main themes: Dynamic NC transition during switching involves altering circuit time constants using resistors or capacitors in series. Steady state NC occurs in complex systems where ferroelectric components integrate with non-ferroelectric materials. Under specific electrostatic conditions, NC stabilizes thermodynamically, minimizing the system`s total free energy.

This study aims to stabilize NC in FE structures by inducing internal electric fields, aligning the system near coercivity. While standalone FE capacitors struggle to stabilize NC without external fields, multilayered thin films offer a promising solution. Typically, FE layers are paired with dielectrics/isolators, and certain configurations demonstrate steady-state NC, often at nanoscale or specific temperature domains. The challenge lies in mitigating large depolarization fields, possibly achievable via bilayer structures with slight polarization discrepancies.

To address this, bilayered structures of two PZT layers with differing properties are constructed, such as p-n heterojunctions using PZT with different doping as Fe, Nb, Bi, or bilayered PZT with different Zr/Ti ratios. Most of these structures exhibit evident amplification of capacitance compared to the equivalent series-connected capacitance, across a large temperature domain. The complex capacitance-frequency characteristic of these structures indicates a complex equivalent circuit. Analysis of these complex circuits compared with simple component layers concludes that at least one of the FE layers in these bilayered structures is in an NC state or very close to this region.

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ORAL PRESENTATION

S4-OP2

High throughput graphene production via intercalation-expansion method

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A widely used route for high yield solution-based graphene synthesis is bulk graphite oxidation/intercalation followed by layer separation, resulting in a highly oxidized graphene and then reduction to graphene. The required oxidation state generally induces a large number of structural defects in the final graphene. Here we report a scalable synthesis method based on H_2SO_4 intercalation for graphite intercalated compound (GIC), followed by energetic exfoliation by microwave exposure under ambient conditions that produces with high efficiency and yield a material consisting of several layers of graphene sheets.

The 2D morphological characterization of the surface was performed by SEM analysis, the chemical composition of the film was identified by EDS and XPS techniques, and the graphene layer and its lateral dimension were determined by AFM analysis based on topographic height images.

NOTES

ORAL PRESENTATION

S4-OP3

Biosynthesised gold nanoparticles: Tunable thermo-plasmonic nanogenerators from visible region to NIR I and II Biological Windows

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Currently, photothermal therapy (PTT) has gained interest due to its ability to treat malignant tumors without causing injury to the healthy cells. This therapy relies on conversion of NIR light energy into heat using photothermal agents. For PTT implementation, a photothermal agent should (i) reach a temperature over 42 °C under irradiation; (ii) be biocompatible and photothermally stable; (iii) be under 300 nm to go undetected by the immune system. Thus, metallic nanoparticles can be modified to complete these requirements [1].

In the present study, we utilize gelatin's dual ability as both a reducing and stabilizing agent for the synthesized gold nanoparticles. Moreover, by modifying the gelatin concentration, we can modulate not only the shape of the nanoparticles, herein nanospheres (AuNSs) and nanotriangles (AuNTs), but also the size which generates tunable LSPR response from visible to NIR region. Since AuNSs are present in the AuNTs solution, one probe of AuNSs was also irradiated for differentiating the temperature contribution of each type of nanoparticle. The colloidal solutions were irradiated with LEDs ranging from visible (405 nm, 530 nm, 660 nm), NIR I (970 nm) and NIR II (1100 nm) for 15 minutes. The highest temperature increase for AuNSs and AuNTs was achieved for 405 nm LED irradiation, approximately 12 °C. Under 530 nm LED excitation, the probes had a temperature increase of 4 °C and 5 °C, respectively. As the LSPR band is positioned further in the NIR region, AuNTs' light absorption decreases. Hence, upon 970 nm and 1100 nm LED irradiation, NIR I AuNTs exhibit an increase in temperature of 2 °C, 1.5 °C respectively, and NIR II AuNTs of 0.5 °C for both sources.

To conclude, AuNTs represent optimal nanogenerators that can be successfully translated into PTT applications.

Reference:

[1] K. Yang, et al., Coord. Chem. Rev. 454 (2022) 214330.

NOTES

ORAL PRESENTATION

S4-OP4

Double electron donor-embedded polymers for energy-efficient smart windows

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In our ongoing quest for advanced materials to address contemporary technological challenges, we have engineered chemical components for constructing new polymers suitable for electrochromic (EC) energy storage applications. Building upon previous investigations [1], this study presents a pioneering approach to develop novel electroactive materials based on phenoxazine (POZ) for integration into electrochromic energy storage (EES) systems. To achieve this, we designed and synthesized a new diamine structure featuring a pendant double electron-donor core by incorporating POZ and diphenylamine (DPA) into the same framework. This structural motif aimed primarily to enhance the electrochemical stability and solubility of the materials. Subsequently, we evaluated the efficiency of the POZ-DPA-based core by employing three distinct polymeric platforms: polyimide (PI), polyazomethine (PAz), and polyamide (PA). Our goal was to identify the most promising performer among these polymers in terms of their electrochemical and electrochromic properties. Structural confirmation of all synthesized organic compounds was conducted using standard spectroscopic techniques, followed by comprehensive physicochemical and computational analyses. The POZ-DPA-based polymer exhibiting the most favorable electrochemical and EC characteristics in the three-electrode cell setup was selected for further investigation. This phase involved constructing laboratory-scale EES prototype devices to assess their performance in terms of both EC and energy storage efficiency and stability, with the aim of unlocking their full applicative potential.

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Reference:

[1] C. P. Constantin, M. D. Damaceanu, Chem. Eng. J. 465 (2023) 142883.

NOTES

ORAL PRESENTATION

S4-OP5

In Vitro hyperthermia with iron oxide magnetic nanoparticles

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Targeted magnetic hyperthermia, a promising approach in cancer therapy, is based on the rising temperature to 40 – 45 °C through an alternating magnetic field (AMF) applied to magnetic nanoparticles (MNPs). It takes the advantage that cancer cells are more sensitive to temperature rise than healthy cells and therefore are preferentially killed in this temperature range. It is known that a tumor is related to hypoxic and acidic conditions following poor vasculature, which could explain the strong susceptibility of a tumor to hyperthermia. Also, cancer cells overexpress different transport membrane proteins that can be used for the selective incorporation of MNPs. Protein selectivity is influenced by a series of MNPs features such as size, hydrophilicity/ hydrophobicity, surface energy, and charge, whereas hyperthermia mechanisms are influenced by size, shape, volume fraction, and type of magnetic material.

The present research investigates magnetite (Fe_3O_4) nanoparticles synthesized by thermal decomposition of organometallic compounds with and without their functionalization for selective target of cancer cells. Scanning and Transmission Electron Microscopy and X-ray diffraction, for morphological characterization, and magnetic measurements (e.g., SQUID magnetometry) for magnetic characterization, demonstrated that the synthesis route provided the desired magnetic and morpho-structural properties, such as high magnetizations, size, shape, and dispersion. To increase the intracellular amount of MNPs for cancer cells, the nanoparticles were functionalized with folic acid since the majority of cancer cells overexpress folic acid receptors on the cell membrane. Fibroblasts L929, as healthy cell line control, and HT29 as a pathogenic model were used and the effect of hyperthermia was evaluated using MTS and LDH assays, and flow cytometry. The time exposure and the AMF intensity were varied as well as the nanoparticles' concentration.

The experiments aimed to obtain the optimal AMF and nanoparticle parameters that can induce apoptosis in HT29 cells and no cytotoxic effect in L929 cells by magnetic hyperthermia.

NOTES

ORAL PRESENTATION

S4-OP6

VO_2 based thermochromic coatings for smart window applications

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An interesting solution to minimize air conditioning ventilation in buildings during the Summer time, is to use the so-called smart windows, able to control heat transmittance in the most efficient way. In this respect, one can consider the coatings of the usual windows by thermochromic thin films, which change their reflectivity at a suitable temperature of the supporting glass, as driven by the solar radiation. The change in reflectivity is accompanied by structural changes, which may lead to observable modifications of other physical parameters of the films, as for example their electric or magnetic properties. A convenient coating for such applications is vanadium dioxide (VO_2) thin film, presenting a reversible phase transition at about 68 °C. Below this temperature, VO_2 shows a monoclinic structure (M1 phase) with insulating behavior. Above this temperature, it undergoes a lattice distortion to a rutile type tetragonal structure (R phase), exhibiting metallic behavior and consequently, increased reflectivity. From the smart window applications, it is this metal-to-insulator transition (MIT) which has to be optimized with respect to the transition temperature as well as to the amplitude, sharpness, cyclicality and reproducibility. To note here the wide structural polimorfs specific to VO_2, each phase being better stabilized under specific deposition conditions as well as the very challenging task to preponderantly stabilize the desired phase susceptible to MIT.

This work reports on the optimization of MIT in coatings based on VO_2 thin films (simple and doped, TiO_2/VO_2 multilayers) obtained by Pulse Laser Depositions (PLD). Different substrates, Oxygen pressures, substrate temperatures and film thicknesses were considered. The optimized coatings, investigated by morpho-structural, electric resistivity, magnetic and optical methods have shown stable and reproducible variations of resistivity by more than 3 order of magnitude and of the reflectivity by tens of percent. The hysteretic transition has been optimized with respect to amplitude, sharpness, wideness and transition temperature. The finest control of the transition temperature was achieved via doping, whereas the control of the amplitude was sensitive to many other geometrical and deposition parameters. A comprehensive discussion on the connections between the morpoho-structural and functional parameters of the coatings is envisaged.

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ORAL PRESENTATION

S4-OP7

Synthesis, characterization and optoelectronic applicability of Sb_2S_3 thin films for enhanced solar energy conversion

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The binary chalcogenide compound antimony sulfide (Sb_2S_3) has garnered considerable interest as a promising candidate for solar applications due to its ideal bandgap of about 1.7 eV, alongside a range of distinctive and beneficial characteristics. Although Sb_2S_3 has fascinating promise as a material for thin-film solar cells (TFSCs), development has been constrained by the deficiencies of reported substrate-configured devices. The unfavorable [hk0] orientations of Sb_2S_3 are the origin of relatively low power conversion efficiencies (PCE<8%), being highlighted in the literature as a key problem. These less-than-ideal results have been made worse by the common approaches for producing Sb_2S_3 absorber layers, primarily physical vapor deposition methods. On the other hand, here basic spin-coating method to deposit Sb_2S_3 thin films onto the FTO substrate coated with a compact TiO_2 electron transport layer is used. Investigating the effects of film thickness, which was varied from 1 to 4 layers, revealed a captivating transformation in the Sb_2S_3 films. This transformation appeared as a change from a nearly amorphous state to a well-defined polycrystalline structure, characterized by the appearance of sizable, and horizontally aligned plate-like grains. The designed substrate-configured TFSCs, constructed as SLG/FTO/TiO_2/Sb_2S_3/HTM/Au devices have PCE lower than 2%, ways to improve the photovoltaic characteristics being also outlined.

NOTES

ORAL PRESENTATION

S4-OP8

Mitigating the toxicity during perovskite solar cell fabrication

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Perovskite solar cells still remain a very interesting and attractive field due to their rapid efficiency growth over the past two decades, attaining a very impressive 25.7% in 2023 [1]. Therefore, researchers have already started looking for solutions to the multiple barriers to commercial implementation. One of the problems to industrial fabrication is the necessity of toxic solvents, namely dimethylformamide (DMF), in the perovskite precursor solution for lead iodide solubilization. Two different less toxic solvents, N-methyl-2-pyrrolidone (NMP) and ethyl acetate (EA) were investigated as candidates for the partial replacement of the main and most toxic solvent - DMF. Standard structured perovskite solar cells using $K_{0.1}FA_{0.7}MA_{0.2}PbI_{2.8}Cl_{0.2}$ (KFAMA) as an active material were fabricated using three solvent mixtures [1]. The effects of the different solvents on the structural, optical and morphological properties of the perovskite layer were analysed by X-ray diffraction, scanning electron microscopy, atomic force microscopy and spectroscopic ellipsometry. Completed perovskite solar cells were characterised by current-voltage measurements, photovoltaic parameters, specifically open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), series and shunt resistances (Rs and Rsh) and power conversion efficiency (PCE) being calculated. The hysteresis factor (Hi) was also determined using the method developed by Nemnes et al. [3], showing a link between the Hi factor and perovskite film quality.

Acknowledgements:

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References:

[1] S. Khatoon, et al., Materials Science for Energy Technologies 5 (2023) 437–459.
[2] V. Stancu, et al., Coatings 13 (2023) 378.
[3] G.A. Nemnes, et al., Sol. Energy 173 (2018) 976–983.

NOTES

ORAL PRESENTATION

S4-OP9

Optical, electrochemical and photovoltaic properties of side chain effects on BDT and TPD-containing polymers

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Due to affordability, ease of manufacturing, adaptability to flexible substrates, excellent film-forming characteristics, high morphological stability, and lightweight properties, organic thin-film photovoltaics (OPV) have garnered significant attention from researchers over the past two decades [1], [2], [3]. Furthermore, the recent advancements in efficiency, particularly attributed to the utilization of non-fullerene acceptors, along with their suitability for indoor photovoltaic applications, suggest that OPVs will continue to be widely utilized in the next years. [4], [5]. Three random polymers P-HBT-T, P-FBT-T, and P-FBT-O were synthesized and employed in this study. The impacts of fluorination and side chains on BDT have been examined for their electrical, optical, and photovoltaic properties. Trap-assisted recombination and bimolecular recombination loss mechanisms, which are pivotal in determining power conversion efficiency (PCE), were examined across all devices.

The photovoltaic investigations involved in-depth optimization, including active layer optimization, followed by morphological and topographic analyses upon completion. Through comprehensive studies, the polymer exhibiting the most promising performance was found to be P-FBT-O, boasting a PCE of 9.21%, a fill factor (FF) of 60.33%, and a Voc of 0.95V [6], thus demonstrating superior photovoltaic capabilities among the polymers examined.

References:

[1] G. Yu, et al., Science 270 (1979)1789–1791
[2] M. Kaltenbrunner, et al., Nat. Commun. 3 (2012) 770.
[3] G. Li, et al., Nat. Photon. 6 (2012) 153–161.
[4] T. P. A. van der Pol, et al., Adv. Energ. Mater. 13 (2023) 2300003.
[5] W. Wang, et al., Joule 7 (2023) 1067–1079.
[6] E. A. Yilmaz, et al., Mater. Today Energ. 36 (2023) 101369.

NOTES

ORAL PRESENTATION

S4-OP10

Acid modified MXENE for PET Depolymerisation

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Polymer recycling has raised environmental concerns that throw a shadow over the usefulness of these materials in our economy and daily life. Heterogeneous catalysis is essential for recycling waste plastics, but none of these have shown excellent performance, hence no industrial strategy has been developed [1,2]. This work envisages novel solid acids that depolymerize PET to raw materials. MXenes, a recently identified group of two-dimensional (2D) metal carbides-nitrides exhibiting graphene-like structures, have gathered significant interest since their unique properties. These materials are synthesized through the etching of A element from the MAX phase [2,3]. Modulating the surface of MXenes presents a potentially valuable strategy for controlling their catalytic activity. In this scope, we have modified MXene with acid groups by adding sulfanilic acid moieties on the MXene surface. Different levels of sulfanilic acid salt were employed to determine the acid group concentration, named as $Ti_3C_2T_x$–SO_3H–y, where y=(1, 3, 5, 7) and represent the amount of sulfanilic acid introduced. Different techniques (XRD, DRIFT, RAMAN, SEM, TEM) showed that the as-modified MXene structure remains lamellar and did not collapse during sulfonation process. The interlayer spacing of the MXene layers increases following modification as a result of the presence of aryl sulfonate groups attached between them. The presence of –SO_3H groups on the MXene surface has been confirmed by the EDX (SEM) and XPS results. These materials converted PET hydrolysis depolymerization into 75% terephthalic acid with no further reaction products. The reaction parameters (temperature, pressure, and catalyst quantity) were also examined, and indicate that $Ti_3C_2T_x$–SO_3H-x is a good candidate for environmentally friendly PET up-cycling.

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References:

[1] D. P Serrano, et al. ACS Catal. 2 (2012)1924-1941.
[2] M. Naguib, et al. Adv. Mater. 23 (2011) 4248.
[3] a) M. Naguib, et al., Acc. Chem. Res. 48 (2015) 128; b) M. Naguib, et al. ACS Nano 6 (2012) 1322.

NOTES

ORAL PRESENTATION

S4-OP11

Continuous hydrothermal flow synthesis of biomass-related carbon quantum dots (CQDs) as nanosensors for carcinogenic ions detection

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Carbon quantum dots are zero-dimensional (smaller than 10 nm) photoluminescent carbon nanoparticles [1]. Discovered in 2004 by Xu et al. [2], since plenty of bottom-up and top-down synthetic methodologies have been established [3]. Developing green and sustainable synthetic routes for the large-scale production of CQDs remains a challenge.

Continuous hydrothermal flow synthesis (CHFS) uses supercritical water as a solvent, which is part of hydrothermal methodologies. CHFS was adjusted for a diversity of nanomaterials synthesis and engineering [4–6]; expanding the portfolio to CQDs is an important step to address the large-scale synthetic challenge. Our research group succeeded in developing CHFS methodologies for carbon quantum dots(CQDs) and nitrogen-doped quantum dots (NCQDs) synthesis from biomass-related carbon sources such as citric acid1 and glucose [7,8]. Considering that all the hexavalent chromium compounds are classified as Group 1 carcinogens by the International Agency for Research on Cancer (IARC)[9], the risk of developing cancer increases with the level of Cr (VI) exposure. Developing sensitive and selective nanosensors for real-time detection of Cr(VI) ions in water is needed.

In this work, we succeeded in synthesising CQDs and NCQDs by developing a faster, greener, and cheaper method than anything available. The as-produced CQDs showed good hexavalent chromium sensibility (LOD: 0.36 ppm) and selectivity.

References:

[1] I.A. Baragau, et al., J. Mater. Chem. A 8 (2020) 3270–3279.
[2] X. Xu, et al., J. Am. Chem. Soc. 126 (2004) 12736–12737.
[3] X. Wang, et al., Front. Chem. 7 (2019) 1–9.
[4] J.A. Darr, et al., Chem. Rev. 117 (2017) 11125–11238.
[5] S. Kellici, et al., RSC Adv. 4 (2014) 14858–14861.
[6] S. Kellici, et al., React. Chem. Eng. 3 (2018) 949–958.
[7] I. A. Baragau, et al., ACS Sustain. Chem. Eng. 9 (2021) 2559–2569.
[8] I.A. Baragau, et al., Chem. Eng. J. 405 (2020) 126631.
[9] The facts: Chromium VI. Roadmap on Carcinogens (2018).

NOTES

ORAL PRESENTATION

S4-OP12

Photocatalytic water splitting using 1D-nanofilaments TiO_2-based lepidocrocite

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Water and sunlight are commonly considered to be the most untainted, exceptionally sustainable, and abundant resources accessible on Earth. Photocatalysts have the capacity to capture solar energy and assist in the process of water splitting into its constituent elements, specifically O_2 and H_2. The latter pertains to a form of ecologically sustainable fuel that is currently under development as a prospective alternative to conventional fossil fuels. The scientific community has long aspired to develop cost-effective and scalable photocatalysts with remarkable stability for H_2 generation. Nevertheless, despite diligent endeavors, there are currently no commercially available resources that meet all the essential requirements for widespread adoption, such as high light quantum efficiency, stability, safety, and affordability. From a cost analysis perspective, the current projection for the production of H_2 using photocatalysis indicates a cost of approximately 10 US dollars per kilogram. The key factor influencing this cost is the photocatalyst itself. Concurrently, the generation of H_2 by the process of fossil fuel reformation, which is widely acknowledged as environmentally unsustainable, results in an expenditure of approximately 1 US dollar per kilogram. Therefore, to attain competitiveness, photocatalysis requires a substantial decrease in its cost, perhaps by a factor of ten or more. This reduction is essential for the achievement of a global economy based on solar energy and H_2.

The results of this study [1] show how to make 1-D nanofilaments (NFs) from lepidocrocite. These NFs have a cross-sectional area of about 5 × 7 A2. NFs possess the capacity to generate H_2 upon exposure to simulated sunlight in a mixture of water and methanol in a volumetric ratio of 80:20. The NFs demonstrated exceptional durability when stored in these mixes for a duration of over 4300 hours, during which 300 hours were dedicated to irradiation. Achieving quantum yields of significant magnitude, specifically 11.7%, was successfully accomplished. The examination of D_2O yields findings that suggest water functions as the primary source of H_2. Additionally, the analysis could not detect any occurrence of CO_2 arising from the photocatalytic degradation of methanol. Therefore, these new materials exhibit the essential properties of a highly effective photocatalyst, such as effective separation of charges, fast transfer of charges, and notably, long-lasting stability in water-based environments. The results of this research offer new possibilities for exploring energy generating systems that employ 1-D NFs created from affordable, environmentally friendly, and readily accessible source materials.

Acknowledgements:
This work was supported by Romanian Ministry of Research, Innovation and Digitization through the Core Program 2023–2026 (contract PC3-PN23080303).

Reference:

[1] H.O. Badr, et al., Matter 6 (2023) 2853–2869.

NOTES

ORAL PRESENTATION

S4-OP13

Portable biosensing devices for healthcare

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Over the past decades, there has been an increasing interest in the development of personalized health care systems such as wearables and point-of-care testing devices capable of detecting chemicals relevant to disease diagnosis [1,2]. Such devices should be able to collect, transduce and interpret the data, as well as to hold the possibility of integration with electronic circuits for data transmission on mobile devices for continuous monitoring. Electrospinning represents a technique which holds the possibility of fabricating polymeric fiber meshes with diameters in the submicron range, by fine tuning the process parameters. The advantages of these materials are represented by their high surface area and flexibility with increased mechanical resistance, while their subsequent metallization enables the fabrication of conductive materials. The integration of these flexible electrodes with polymeric fluidic supports, their functionalization with bio- and biomimetic-molecules, as well as their applications for sensing ions, small molecules and nucleic acids is described [3–6].

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References:

[1] D. Botta, et al., Curr. Opin. Electrochem. 42 (2023) 101418.
[2] R.J.B. Leote, et al., Curr. Opin. Electrochem. 34 (2022) 101024.
[3] V.C. Diculescu, et al., Sci. Rep. 9 (2019).
[4] A. Aldea, et al., Electrochim. Acta 363 (2020) 137239.
[5] A. Aldea, et al., Microchem. J. 165 (2021) 8–11.
[6] R.J.B. Leote, et al., ACS Appl. Polym. Mater. 6 (2024) 2274–2283.

NOTES

ORAL PRESENTATION

S4-OP14

Electrochemical impedance spectroscopy based biosensors for bleomycin detection

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Bleomycin is a chemotherapy drug used in several types of cancer, with serious pulmonary and other adverse effects. Because the exact mechanism of action is not yet known, to reduce side effects a better understanding of the pharmacodynamics of bleomycin is needed. This research validates two types of electrochemical impedance spectroscopy-based biosensors capable of detecting very low concentrations of bleomycin that can be used to study its binding to DNA. The first sensor is a silicon-based gold interdigitated electrode enhanced with vertical graphene (VG-IDE). The second is a 3D-printed electrochemical sensor (3D-PES). Both sensors have been functionalized with DNA probes. We compared different electrical parameters of the two sensors to assess which one is more suited for pharmacodynamics studies. After applying 10 µl of bleomycin (10 mM), the VG_IDE sensor exhibited a charge transfer resistance (Rct) of 106 (ohm) and polarization resistance (Rp) of 226 (ohm), indicating high sensitivity. Under the same measurement conditions, the 3D-PES exhibited Rct = 292 (ohm), and Rp = 474 (ohm), respectively. Both sensors have their advantages and disadvantages: the VG-IDE demonstrates high sensitivity but requires a complex technological process and has an estimated price of 10 euros, while the 3D-PES offers a much simpler and faster fabrication process, with an estimated cost of 2 euros, albeit with slightly lower sensitivity compared to the VG-IDE. At this point, either sensor can effectively detect 10 mM of bleomycin. Further investigations will determine which sensor is more suitable for pharmacodynamic studies.

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ORAL PRESENTATION

S4-OP15

Micro 3D and 4D printing of pH-sensing multi-material microrobots

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Microrobots have shown great promise for biomedical applications such as cargo transport, assisted fertilization or sensing [1]. For microrobot fabrication, two-photon polymerization (2PP) is the 3D printing technology with the highest resolution. By 2PP, it is possible to fabricate polymer structures with complex shapes, overhanging features, critical dimensions of a few hundreds of nanometers and total sizes up to several millimeters [2,3].

Here, we present the fabrication, characterization and actuation of multi-material microrobots comprising a 3D printed hard polymer backbone and 4D printed pH-responsive hydrogel sensing elements. The microrobot designs were conceptualized based on two main considerations. The first is that a user should be able to identify visually when the sensing element changes size, which happens as the microrobot encounters the target analyte. The second is that the microrobots should be manipulated using optical trapping [4], which require the presence of spherical structural elements with a good refractive index contrast to water. These requirements make it necessary to include a smart material for the sensing element, as well as an inert material for optical trapping and for size referencing.

The microrobots are fabricated by 2PP. First, hard polymer backbones are printed using the IP-L commercial photoresist, together with alignment markers for subsequent processing. After development, the custom hydrogel formulation is added to the substrate. An image of the hard polymer backbones is taken and an algorithm using binary thresholding, Canny edge detection and a circle Hough transformation is applied to perform rotational and translational alignment. Then, the hydrogel sensing elements of the microrobots are printed on top of the hard polymer backbones. The micro-robots are then transferred to a microfluidic cuvette integrated into an optical trapping setup for sub-sequent pH measurements.

The optimal fabrication parameters for the custom pH-responsive photoresist are determined using design of experiments. The criteria for optimization are i) the size change from acidic to neutral pH, and ii) the size match between the 3D design and the printed structure. In this manner, we obtained robust sensing elements with a 35 % size increase from acid to neutral pH.

To conclude, multi-material microrobots for localized pH sensing were fabricated using a two-step fabrication process with automated alignment. The microrobots were successfully trapped and manipulated using a custom optical trapping setup. Future work will focus on characterizing the sensitivity of the microrobots to pH changes, and on localized pH measurements in both batch and microfluidic setups.

NOTES

ORAL PRESENTATION

S4-OP16

Advanced functional materials as trigger for fibroblasts differentiation and wound healing stimulation

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The wound healing process is usually characterized as four sequential but overlapping phases: haemostasis, inflammation, proliferation and remodeling. Deregulation of any of these steps results in impaired healing, e.g., chronic hard-to-heal ulcers or excessive scarring, which presents a major and increasing health and economic burden to our society. Fibroblasts are important players in regulating tissue homeostasis and are involved in wound healing, where they differentiate into contractile myofibroblasts leading to wound closure. In nonhealing chronic wounds, fibroblasts fail to undertake differentiation. Thus, the control of this process represents a step forward in healing management of chronic wounds.

The aim of our work is to develop functional materials able to trigger fibroblast differentiation without applying any kind of external stimulus, and that can be used as smart bandages to accelerate the healing of chronic wounds. Thus, polymeric electrospun nanofibers, before and after modification with conductive polymers PEDOT:PSS, and graphene as double- and multi-layers, were used as scaffolds to evaluate the adhesion, proliferation and differentiation of fibroblast cells in myofibroblasts. Scanning electron and fluorescence microscopy, and Raman and UV-Vis spectroscopy were used for morphological characterization. Immunofluorescence assays, using vinculin and alpha smooth muscle actin fluorescent antibodies were chosen for investigation of adhesion and differentiation processes. The in vitro studies using L929 fibroblast mouse cells showed that the bioactive materials have no cytotoxic effect and allowed cell adhesion and proliferation. Also, the results obtained sustain the aim that the scaffolds substrates used in these studies have the potential to induce the differentiation of fibroblast cells into myofibroblasts, showcasing its favorable effects on cell behavior and function. Overall, this investigation introduces an innovative and effective method for employing electrospun polymeric nanofibers as well as graphene layers, with tailored properties, significantly augmenting their suitability for advanced healthcare applications, mostly in areas dealing with biologic/synthetic interfaces.

NOTES

ORAL PRESENTATION

S4-OP17

Saturation and stability tests of chalcogenide-porphyrin nanocomposite for methane sensing at environmental temperature

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Methane sensitive nanocomposite thin films working at room temperature (25–30 °C) have been prepared, starting from $SnSe_2$ powder and Zn(II)-5,10,15,20-tetrakis-(4-aminophenyl)-porphyrin (ZnTAPP) powder. The film deposition was made by drop casting from a suitable solvent for both starting materials, after mixing them in an ultrasonic bath. SEM images were used to estimate the thickness of these films, which were found to be around 1.2 µm. These thin films proved to be sensitive to a threshold methane (CH_4) concentration as low as 1000 ppm, at a room temperature of about 25 °C, without the need for heating the sensing element. The nanocomposite gas sensing material has a prompt and reproducible response to methane in dry air, and in the presence of air with 50% relative humidity (RH) as well. It is suitable for signaling gas presence before reaching the critical lower explosion limit concentration of methane at 50.000 ppm.

Here we address saturation and stability tests of the nanocomposite, alternating the presence of the test gas for a longer time compared to our earlier studies.

NOTES

ORAL PRESENTATION

S4-OP18

Fabrication of a portable electrochemical cell based on flexible porous materials

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Over the past decade, there has been a growing interest in the development of portable sensing devices based on porous substrates such as paper or textiles, primarily due to their ability to passively transport fluids by capillary action. While screen-printing represents a straightforward and cost-effective technique for fabricating the electrodes, the major drawback comes from the low degree of reproducibility [1]. Recent studies shown that metallized electrospun polymeric fiber meshes could serve as promising alternatives for flexible electrodes in various sensing applications, due to their high surface-to-volume ratio [2]. This study describes the techniques involved for successfully integrating metallized electrospun fiber meshes with chromatographic paper for the development of a reliable portable electrochemical cell. Two important steps of the fabricating procedure consisted of patterning the paper into hydrophilic and hydrophobic areas, and the fiber meshes into conductive/non-conductive regions, which could be achieved by 3D printing. While fused-modelling deposition from polymeric materials with low melting points provided a means for creating hydrophobic barriers, sputtering masks stable in vacuum pressure could be fabricated by stereolithography with photopolymeric resin. Another key factor in the design of a reliable electrochemical platform is represented by the uniformity and integrity of the electrodes' structure. Thus, the process and environmental parameters which lead to uniform electrospun polymeric fiber meshes with reproducible characteristics were evaluated. The conductivity of the fibers was achieved by sputtering deposition of metals such as gold, silver, platinum, or palladium and their morphology before and after the attachment to the chromatographic paper was analyzed by scanning electron microscopy. Multiple architectures of the electrochemical cell designed in two and three electrode configurations were studied and the performance of the assembled device was investigated by cyclic voltammetry and electrochemical impedance spectroscopy in the absence and in the presence of redox probes. As a proof of concept, detection and quantification of enzymatic reaction by-products such as H_2O_2 and NADH, as well as glucose in the presence of glucose oxidase, and nucleic acids with or without makers were performed using the fabricated electrochemical cell.

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References:

[1] D. Botta, et al., Current Opinion in Electrochemistry 42 (2023) 101418.
[2] R. J. B. Leote, et al., ACS Appl. Polym. Mater. 6 (2024) 2274–2283.

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ORAL PRESENTATION

S4-OP19

Designing ptohosensitizers based on some derivatives of Zinc Phtalocyanine

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In the last time, the designing of new photosensitizers for anticancer photodynamic therapy and photodynamic antimicrobial chemotherapy with good solubility, stability in biological media, excellent biocompatibility, absorption in the appropriate NIR region, triplet state and improved singlet oxygen generation has attracted considerable research in the pharmaceutical field. This presentation is dedicated to the optimization of the synthesis of metal zinc phthalocyanine (ZnPc) derivatives with functional groups specific to the biomolecules of the human body, using the method of microwave irradiation of the reactant mixture, the classical method and to the modification of the surface of the noble and magnetic nanoparticles with different hydroxy groups, polymers and conjugation with metal phthalocyanine derivatives. Also, spectral evaluation (absorption, fluorescence) of synthesized photosensitizers in aqueous solutions with different polarities, accepted for pharmaceutical formulation and evaluation of the lifetime, the quantum yield of fluorescence and phosphorescence of new synthetized photosensitizers are presented. Substitution of the periphery of ZnPc with carboxy, thiol, OH groups increases water solubility. Zinc phthalocyanine [phthalocyaninato]zinc oktakis (methyl isothiuronium) chloride (MeIt)8ZnPcCl8 and zinc phthalocyanine derivative with eight thiol groups (HSMe)8ZnPc were synthesized based on ((ClMe)8ZnPc) obtained by chloromethylation reaction of ZnPc.The best triplet quantum yields of 3.35% for (MeIt)8ZnPcCl8 in 1NVP:9H_2O solution and 14.35% in water were reached. All synthesized compounds of ZnPc derivatives with tetra and octa carboxy group show a high molar extinction coefficient (2-8) 104 M−1·cм−1 in DMSO:H_2O. From all synthesized ZnPc derivatives with carboxy group, the photosensitizer based on $ZnPc(COOH)_4$ conjugated with Fe_3O_4 nanoparticles coated with chitosan (CH) has the best photophysical properties because some photophysics parameter are better compared to commercial Photosens based on sulfonated form of AlPc. Absorption peak for $ZnPc(COOH)_4/Fe_3O_4$/CH compound is in the range of 700–702 nm, while for commercial Photosens is observed at 678 nm. In the case of the $ZnPc(COOH)_4/Fe_3O_4$/CH photosensitezer, values of the triplet quantum yield of 56 % and the lifetime of the triplet excited states of 1.6 µs and 12.3 µs were achieved. The obtained $ZnPc(COOH)_4/Fe_3O_4$/CH composite showing much better lifetime of the triplet excited in contrast to Photosens with $\tau1 = 0.68$ ns and $\tau2 \approx 5$ ns [1]. This comparison of $ZnPc(COOH)_4/Fe_3O_4$/CH composite with commercial Photosens compels us to in vitro and in vivo studies.

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References:

[1] A. Brilkina, et al., Journal of Photochemistry and Photobiology B: Biology 191 (2019) 128–134.

NOTES

ORAL PRESENTATION

S4-OP20

Strategies to improve the mechanical and thermal features of silica aerogels for thermal insulation applications

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For effective thermal insulation applications, materials with reduced weight that combines both good thermal insulating and mechanical properties are required. In this sense, silica-based aerogels with mesoporous network (>90% porosity), low density (<150 kg m^{-3}), low thermal conductivity (0.015 – 0.025 W m^{-1} K^{-1}) and non-flammable character are excellent candidates as thermal insulators in buildings, protective suits, aerospace [1,2].

Despite their exceptional properties, pure silica aerogels also present some drawbacks, like brittleness and hydrophilic behaviour, which limit their application on a large-scale, especially as monoliths.

Herein, some alternatives to overcome the mentioned issues will be presented, including reinforcement by organic thermally stable fibers (aramid) [3] and introduction of a higher dimensional thermal stability refractory phase (alumina) [4].

For increasing the robustness of the aerogel´s structure and maintain its monolithicity, different para- and meta-type aramids, including short pulp, long fibers, and felt, were incorporated into the silica matrix [4]. Generally, the para-type fibres produce stiffer composites with best insulation performance. Furthermore, to enhance the contact with the gel matrix at microscopic level and achieve a more balanced response when submitted to stress loads, the reinforcement with mixtures of aramid nanofibres and microfibres was also investigated, which led to the improvement of the mechanical properties by a factor of 3 [5].

To overcome the densification of silica aerogels at higher temperature and improve their performance in these environments, small amounts (up to 15 mol%) of alumina phase (aluminum chloride and tri-sec-butoxide) was introduced in the nanocomposites [3]. The aerogels with aluminum chloride were much more promising, with lower densities (130 kg m^{-3}) and thermal conductivities (30 mW m^{-1} K^{-1}).

The practical application of the composite aerogels was verified through simulated tests (thermal cycling and outgassing) in conformity with Space conditions and the scale-up process of the optimized nanocomposites was also performed [4,5].

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References:

[1] F. Akhter, et al., J. Porous Mater. 28 (2021) 1387.
[2] T. Linhares, et al., J. Mater. Chem. A 7 (2019) 22768.
[3] M.E. Ghica, et al., J. Sol Gel Sci. Technol. 101 (2022) 87.
[4] C.M.R. Almeida, et al., J. Mater. Sci. 56 (2021)13604.
[5] M.E. Ghica, et al., L. Durães, Gels 9 (2023) 535.

NOTES

ORAL PRESENTATION

S4-OP21

Strategies to improve the mechanical and thermal features of silica aerogels for thermal insulation applications

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In general, target gases react with the surface of the heated metal oxide semiconductor gas sensor and are consequently converted into different products depending on the target gas and sourounding conditions. Under normal air conditions, for example, reducing gases such as CO and H_2 are oxidized to reaction products forming: CO_2 and H_2O by reaction with pre-adsorbed oxygen species from the surface of the gas-sensitive material (generally considered to be at the origin of the gas sensor response). A powerful and simple method that allows us to get insights about the reaction pathways and the mechanisms that take place during these reactions is therefore to measure the variations in the composition of the ambient atmosphere caused by the detection process. Basically, the gas composition before and after the sensor chamber is monitored. Herein, an INNOVA 1314 photoacoustic analyzer equipped with optical filters for CO, CO_2, H_2O and CH_4 was involved. For the simplicity of determining possible mechanisms of interaction with the surface of NiO-based gas sensors, we used carbon monoxide as target gas in the absence and presence of relative humidity. From the simultaneous measurements of electrical resistance and catalytic conversion we were able to decouple between different reaction pathways specific to the intrinsic properties of the NiO sensitive material.

NOTES

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POSTER PRESENTATIONS

(PP)

POSTER PRESENTATION

S1-PP1

Al-doped $SrTiO_3$ photocatalyst with increased performance

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Our research explores the enhanced photocatalytic activity of $SrTiO_3$ in Al-doped $SrTiO_3$ system [1]. We adapted the synthesis method in order to produce well-crystallized materials with low defect density. We employed surface modification techniques in order to improve the photocatalytic efficiency of $SrTiO_3$ by doping with Al_2O_3 nanoceramic oxide at concentrations ranging from 0 to 10%. We investigated the relationship between the doping process and changes in the electronic and crystalline structure of $SrTiO_3$ with three different dopings: Al3%:$SrTiO_3$, Al7%:$SrTiO_3$, and Al10%:SrTiO3. In order to evaluate the stoichiometry (X-ray photoelectron spectroscopy), local environment, and chemical state (X-ray absorption spectroscopy) in total electron yield (TEY) and fluorescence yield (TFY), complementary X-ray techniques were used. The detailed characterization sheds light on the structural alterations brought about by Al doping in the $SrTiO_3$ perovskite lattice and brings a more solid understanding of the changes in the electrical properties and morphological characteristics of the modified samples. This clarifies the surface formation mechanism, showing that the photocatalytic O_2 evolution activity is enhanced by Al alteration of the perovskite structure and that there is an optimum value for the doping which maximizes the efficiency of the photocatalyst.

Acknowledgments:
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Reference:

[1] I. Radu, et al., Ceramics International 50 (2024) 20664–20675.

POSTER PRESENTATION

S1-PP2

Bulk graded (Ba,Sr)TiO_3 structures with enhanced thermal stability

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Here is a comprehensive overview of the results obtained from our research performed on graded structures with various designs. The potential of ferroelectric graded structures to enhance ferroelectric, piezoelectric, pyroelectric, and dielectric properties has generated significant interest. A new approach employing spark plasma sintering was used to manufacture asymmetric and symmetric graded ceramics of BST type, with a gradient in the Sr content. The ceramics were produced from $(Ba_{1-x}Sr_x)TiO_3$ (BST, x = 0.10; 0.20; 0.30) powders. A variation in composition is accompanied by a variation in grain size across the cross-section of the samples, as shown by the structural, microstructural, and chemical analysis. Structural and compositional investigations, including X-ray diffraction, electron microscopy combined with energy dispersive X-ray spectroscopy, were employed to validate the concentration gradient. When discussing pyroelectric detectors, it is important to consider not only the magnitude of the pyroelectric coefficient but also their thermal stability. The pyroelectric coefficient and the dielectric constant both have an impact on this stability. The study revealed that there is an opposite relationship between the number of component layers and the magnitude of the dielectric constant. The dielectric losses are low on the symmetric-graded structures with the highest number of layers, which have the best thermal stability.

The pyroelectric signal is enhanced for frequencies above 100 Hz in symmetric structures, as a result of the combined effects of signals originating from layers with varying Sr content. The pyroelectric signal provides a drop as the temperature of the sample increases, followed by a subsequent recovery upon cooling of the sample to the room temperature. The behavior can be attributed to the internal electric fields caused by phase transitions in the component layers. These transitions induce changes in lattice properties, strain, dielectric constant, and polarization.

POSTER PRESENTATION

S1-PP3

Thermal drift in $Ba_{1-x}Sr_xTiO_3$/polyethylene composites studied by broad-band dielectric spectroscopy

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$Ba_{1-x}Sr_xTiO_3$ (BSTx) is a continuous solid solution between $BaTiO_3$ (BT) and $SrTiO_3$ (ST) across the entire concentration range. The Curie temperature decreases almost linearly with the increasing concentration of ST, allowing for the tailoring of ferroelectric properties. [1]. Polymers offer several advantages such as lightweight, mechanical flexibility, low dielectric loss, and high dielectric strength. Nonetheless, their low relative permittivity limits their use in electrical device manufacturing. Therefore, the formation of polymer-based ferroelectric composites has been extensively investigated for various applications [2]. Here, we report on the fabrication and temperature-dependent dielectric properties of BST/polyethylene composites. Single-phase $Ba_{1-x}Sr_xTiO_3$ (x=0.05, 0.1, 0.15, 0.2, 0.5) powders obtained by solid –state reaction at 1300 oC were mixed with commercial polyethylene (PE) powder. "PE-BSTx" disks with 10%, 50%, 75%, and 90% mass percentages of BSTx were obtained by pressing the mixtures at 150°C for 3 minutes and subsequently painted with silver paste. The broad-band frequency behavior (1 Hz to 10 MHz) of the "PE-BSTx" capacitors was carried out using the Alpha Analyzer from Novocontrol in a range from -40°C to 85°C (standard industrial range). It was found that the relative permittivity of the composites is more sensitive to the BSTx loading level than to the Sr content. Due to the structural phase transitions in the BT-ST system [3], the temperature coefficient of capacitance exhibits a non-monotonic behavior for composites based on BSTx ferroelectric compositions (x=0.05, 0.1, 0.15, 0.2). In general, the thermal expansion of the composites makes the main contribution to the temperature coefficient of capacitance. The dielectric spectroscopy data are discussed in relation to the microstructure of the composites and compared with the results obtained for bulk BSTx ceramics.

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References:

[1] H.V. Alexandru, et al., Applied Surface Science 253 (2006) 354.
[2] F. Gao, et al., Progress in Materials Science 121 (2021) 100813.
[3] L. Nedelcu, et al., Thin Solid Films 519 (2011) 5811.

POSTER PRESENTATION

S1-PP4

Morphological and phase examination of mullite based ceramics developed using synthesized amorphous silica from rice husk ash

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This research examines the preparation of mullite based ceramics using amorphous silica recycled from rice husk ash (RHA) as alternative source of silica by microwave sintering. The aim is to reduce environmental pollution and convert waste to wealth for industrial application. The recycled waste was characterized to determine Phases, morphology and elemental composition present using, XRD, X-ray fluorescence (XRF) and scanning electron microscope (SEM). The mullite based ceramics were produced by varying percentage composition of the materials and sintering at 1200°C for 3hours. The developed samples were characterize using XRD, SEM, FTIR, hardness and compression test while physical test like porosity and bulk density were also conducted. The XRF result of amorphous silica from RHA shows 91.325% of SiO_2 while Al_2O_3, CaO, K_2O has 2.447%, 1.845% and 1.547% respectively. The XRD results of developed samples shows increase in mullite phases as percentage composition of amorphous silica increased while FTIR results reveals enhanced bond formation that denotes cohesion of amorphous silica with other constituent materials. The porosity and density test show that % porosity of samples reduces with increase in amorphous silica while the entire sample shows a reduction in porosity level when compared to the control sample. The samples also showed lower density than the control samples with the highest density value. The SEM images also revealed a uniform particle distribution of materials with the microstructure.

POSTER PRESENTATION

S1-PP5

Sr and Ga doped barium titanate piezoceramics for osteogenic applications

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Inducing faster healing of bone tissue affected by illness or trauma necessitates a multidisciplinary approach. The exploration of cationic substitutions in barium titanate (BT)-type ceramics aimed to achieve a synergistic chemical [1] and piezoelectric [2,3] stimulation of osteogenesis. In this regard, doping with Sr and Ga could enhance both the piezoelectric and osteogenic responses, while also potentially exhibiting angiogenic, antimicrobial, or anticarcinogenic properties. The research focused on studying eight compositions of barium titanate-type materials doped with Sr or Ga, with the stoichiometric formulas $Ba_{1-x}Sr_xTiO_3$ or $Ba_{(1-3x/2)}Ga_xTiO_3$ respectively, where x = 2, 4, 6, and 8. Solid-state synthesis was employed to obtain the ceramics. Mixed raw materials were calcined at 1100°C, followed by milling and sintering at 1400°C for 20 minutes and then at 1350°C for 3 hours. The two-step sintering process enabled obtaining BT ceramics with controlled grain growth and a tetragonal single phase, as evidenced by XRD characterization. SEM investigations revealed grain dimensions of approximately 20 μm for all materials doped with Ga, as well as for materials doped with 2 mol% and 4 mol% Sr. However, materials doped with 6 mol% and 8 mol% Sr exhibited reduced grain dimensions of around 5 μm. The ferroelectric measurements showed that for Ga-doped materials, losses due to conduction at high electric fields increase with the doping level, which is associated with a decrease in density. The highest value of remnant polarization for Sr-doped BTs was measured at 4 mol% Sr, with a value of 15 $\mu C/cm^2$ being obtained. Planar coupling factor kp and piezoelectric constants d33 and d31 tend to decrease with increasing Ga content. The best electromechanical and piezoelectric responses were obtained for the 4 mol% Ga BT. For Sr-doped BT ceramics, the coupling factor and piezoelectric constants decrease with increasing doping level, with the best properties observed for doping with 4 mol% Sr. An increase in compression resistance was observed in the BT doped with Ga 4 mol% (with~26%), Sr 4 mol% (with ~70%) and Sr 6 mol% (with~19%), compared to pure BT. The concentration of Sr and Ga ions released in cellular media was determined by ICP-MS, revealing that they are released in small quantities (<1 mg/L). MTS assays indicated good cell proliferation for all doped BT-type materials. LDH tests showed no detrimental increase in cellular death compared to control, irrespective of type of BT ceramic. Cells with normal morphology and nuclei dimensions were observed for all BTs, with a typical tendency to extend filopodia and lamellipodia.

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The authors thank to the Core Program, project PC1-PN23080101.

References:

[1] V.M. Schatkoski, et al., Ceram. Int. 47 (2021) 2999–3012. [2] A.K. Ulstrup, Acta Orthopaedica Belgica 74 (2008) 291–302. [3] Y. Uto, et al. PLoS One 12 (2017) e0189893.

POSTER PRESENTATION

S1-PP6

Terahertz-Time-Domain Spectroscopy for heavy metals detection in soil

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Currently, several optical and electrical techniques are known that are used in the generation of THz waves. Most pulsed THz sources are based on the excitation of various materials using ultrashort laser pulses. Spectroscopy with electromagnetic waves in the THz domain was introduced to identify the chemical composition of opaque materials, as an alternative to the other spectral domains.

The method used in terahertz radiation spectroscopy is similar to the method used in classical spectroscopy. The aim of this work was the identification of copper sulfate in different soil samples and the establishment of a dependence of the Cu concentration on the transmission of the soil, using THz spectroscopy. The measurements were performed in the frequency range 0.1-4THz, at a maximum number of points (2048), for maximum resolution and a temperature of 220C. As a procedure, we followed every standard step for measurements with the THz-TDS system, that is, after finding the maximum signal and the pulse emitted by the photoconductive antennas, we measured the transmission of the polyethylene container that we use as a reference every time, for the samples of soil and contaminated soil.

Spectra of the samples are obtained by dividing the transmission spectrum of the sample by that of the reference. We measured the samples three times, the presented result being the average of the obtained spectra. I also measured the transmission spectrum of $CuSO_4$, having as a reference the entire transmission spectrum of the polyethylene support, to be able to identify it in the contaminated soil spectra.

POSTER PRESENTATION

S1-PP7

Composites based on polydiphenylamine and multi-wall carbon nanotubes functionalization with carboxylic acid groups for applications in energy storage

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Composites based on polydiphenylamine (PDPA) and multi-wall carbon nanotubes functionalized with carboxylic acid groups (MWNT-COOH) were prepared by the interaction of: a) the PDPA in emeraldine base (PDPA-EB) with MWNT-COOH and b) PDPA in emeraldine salt (PDPA-ES) with MWNT-COOH. Using FTIR spectroscopy and Raman scattering, we demonstrate that: a) the interaction of PDPA-EB with MWNT-COOH leads to synthesis of composites containing PDPA doped with MWNT-COOH, while the interaction of PDPA-ES with MWNT-COOH results in composites based on MWNT-COOH non-covalently functionalized with PDPA-ES. The composites obtained through the two different synthesis, as electrode materials in the energy storage devices, were tested using cyclic voltammetry studies. The presence of the IR band peaked at 1650-1680 cm^{-1} assigned to the vibrational mode of the protonic acid structure within the composites, prepared by the two methods, is reported [1,2]. As increasing of the PDPA-ES weight in the composites mass, the intensity of the Raman line localized at 1300-1400 cm-1 attributed to the vibrational mode of the radical structure of the semiquinone is observed [3,4]. The information concerning the orientation of conjugated polymer onto the MWNT-COOH surface will be shown by anisotropic photoluminescence studies. The preparation of electrodes containing the PDPA/MWNT-COOH composites as active materials in electrochemical cells in the two electrodes geometry and the Nafion membranes activated with H_2SO_4 solution as electrolyte [5] are used for assessing the capacitive behavior of the type of electric double-layer capacitors (EDLC), pseudocapacitive or battery. In this order, the dependence of the current densities with the scan rate of the cyclic voltammograms, within the potential range (-200; +950) mV, will allow to estimate the contribution of the capacitive and diffusion processes. The dependence of the supercapacitors capacitance with the scan rate of the potential and the number of cyclic voltammograms will be shown, too.

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References:

[1] M. Baibarac, et al., Scientific Reports 9 (2019) 11968.
[2] S. Quillard, et al., Phys. Rev. B 50 (1994) 12496.
[3] M. Baibarac, et al., Coatings 11 (2021) 258.
[4] M. Lapkowski, et al., Macromolecules 28 (1995) 1233.
[3] M. Baibarac, et al., Diamond and Related Materials 32 (2013) 72.

POSTER PRESENTATION

S1-PP8

Composites containing poly(vinylchloride) for applications as SERS supports and membranes used in filtration processes

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This communication reports synthesis as well as the optical and morphological properties of composites of the type poly(vinylchloride)/gold nanoparticles (PVC/Au) [1], poly(vinylchloride)/graphene oxide (PVC/GO) [2] poly(vinylchloride)/graphene oxide (PVC/RGO). The PVC spheres were synthetized at 60 Celsius degrees by the interaction of PVC grains with lauroyl peroxide and ethyl cellulose [2]. The ability of these composites to be used as surface enhanced Raman scattering (SERS) supports and membranes used in the filtration processes will be highlighted, too. In this context, membranes based on PVC and the PVC/GO and PVC/RGO composites were prepared using the phase inversion method [3]. A brief characterization of PVC spheres and their composites were highlighted by studies of Raman scattering and FTIR spectroscopy [1, 2]. These studies indicated, simultaneously, a partial dehydrogenation of PVC and the presence of new bonds C-OH and -COO-, in the presence of GO [3]. The ability of membranes based on PVC and their composites is demonstrated by the filtration of the anti-pyretic drugs solutions that were degraded in the presence of UV-light and the titanium dioxide/RGO photocatalysts [1]. In order to prepare SERS supports, the deposition of the colloidal dispersion of Au nanoparticles on the membrane surface by spraying, followed by a fusion process of inorganic nanoparticles achieved by a thermal treatment was applied. The performance of these SERS supports was demonstrate using TiO_2/RGO photocatalysts after degradation of anti-pyretic drugs solutions [1]. The presence of the Raman lines, peaked at 145, 1302 and 1599 cm^{-1} assigned to the Eg vibrational mode in TiO_2 A [4], the breathing vibrational mode of the carbon hexagonal rings [5] and the E_{2g} phonon mode of RGO [5] proves the PVC/Au supports can be used in SERS spectroscopy.

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References:

[1] M. Daescu, et al., Molecules 28 (2023) 4546.
[2] M. Baibarac, et al., Polymers 13 (2021) 565.
[3] A. Bihran, et al., Chim. J. Chem. Eng. 26 (2018) 715.
[4] V. Vaiano, et al., Catalysis Today 230 (2018) 315.
[5] S. Eigler, et al., Carbon 50 (2012) 3666.

POSTER PRESENTATION

S2-PP1

Investigation of the insulator layer role in polarization direction stability in multilayered heterostructures

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Ferroelectric materials have shown great promise in solving current technological problems such as faster and more efficient transistors, energy storage devices and memory devices, to name but a few. All these applications make use of a unique concept proposed more than a decade ago and controversially named negative capacitance. Since then, numerous studies have sought to enhance this phenomenon and harness it for device applications. The common trait of all proposed structures is the interface of one (or more) ferroelectric layers with insulators. This appears either as a design requirement or accidentally during the growth process when thin insulator layers may appear at interfaces with ferroelectric layers. It has been shown that the insulator layer plays a very important role of more than just a separator, contributing to the stability of the ferroelectric polarization itself and influencing the hysteresis curve of the device. For this reason, it is important to study the behavior of ferroelectric layers in the presence of various insulator layers with different conditions such as interface termination and layer thickness. In the current study, several ferroelectric based heterostructures have been fabricated and examined using experimental techniques such as hysteresis polarization-voltage (P-V), piezoresponse force microscopy (PFM) measurements. In addition, density functional theory (DFT) formalism was used to investigate the in-depth influence of the insulator layer on the ferroelectric polarization. It was shown that the state where the polarization direction is towards the insulator layer is more energetically stable than the opposite direction in a metal-ferroelectric-insulator-metal (MFIM) heterostructure. There is a direct contrast with the classical metal-ferroelectric-metal (MFM) capacitor setup where both states are exactly equivalent. In addition is was show that the stability of the two polarization states is also affected by the termination of the ferroelectric layer. The influence of the ferroelectric layer termination affects not only the stability of the polarization states but also the magnitude of the achieved polarization itself.

POSTER PRESENTATION

S2-PP2

Wurtzite III-V materials for ferroelectric component in heterostructures

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Ferroelectrics are crucial components for a wide spectrum of applications, including optoelectronics and non-volatile memories. A new promising ferroelectric materials category is represented by the III-V wide band-gap semiconductors, namely solid solutions of AlN and ScN (Al1-xScxN - ASN). The interest for these materials is emerging due to their high polarization, high coercive field, compatibility with CMOS technology, fast switching speed [1-3]. The correlation between nitrides and ferroelectricity generates a high degree of novelty topic and paves routes towards complex applications of III-nitrides. Nevertheless, for this type of functionality of AlN - based materials, complex analysis needs to be performed in order to understand materials behavior and to drive the depositions towards achieving proper characteristics.

Reported ASN materials with ferroelectric feature were mainly prepared by magnetron sputtering (either DC of RF), but also by molecular beam epitaxy. Sputtering technique is more feasible to translate the ASN preparation process into industrial CMOS micro/nanotechnologies.

In this study, we tested pristine AlN and ASN solid solutions deposited by reactive RF magnetron sputtering techniques on silicon substrates. For electrical characterization, the AlN-based films were integrated in capacitor geometries with platinum top and bottom electrodes. Electrical properties of the these heterostructures were investigates with respect to AlN morphology, structure and composition.

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References:

[1] S. Fichtner, et al., J. Appl. Phys. 125 (2019) 114103.
[2] X. Liu, et al., Nano Lett. 21 (2021) 3753.
[3] K.D. Kim, et al., Adv. Electron. Mater. 9 (2023) 2201142.

POSTER PRESENTATION

S2-PP3

Swinging molecular adsorption of carbon monoxide on ferroelectric $BaTiO_3$(001)

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Carbon monoxide (CO) is reversibly adsorbed and desorbed from ferroelectric (001) oriented, BaO-terminated barium titanate providing permanent polarization and molecular fixation [1–3]. Adsorption proceeds on different sites/geometries as function of the substrate temperature. The system is studied by X-ray Photoelectron Spectroscopy with the use of synchrotron radiation at different photon energy (650, 390, 200 eV) followed by LEED patterns on the clean/absorbed surface. Voigt functions were used in order to "deconvolute" the XPS spectra to analyze the surface at a chemical level [4]. Below room temperature, CO is adsorbed atop on surface Ba. At room temperature, the adsorption proceeds atop on surface oxygen, while at high temperature a "hollow" site adsorption is derived, with carbon coordinated with three oxygens, the initial one and two oxygens from the substrate. The amount of CO adsorbed is about one molecule for 10 surface unit cells, slightly increased at low temperatures. CO is desorbed if the substrate is heated above the Curie temperature [5], which is a sign of the definitory role of ferroelectric polarization. The surface is cleaned by repeated heating in oxygen by electron bombardment and the BaTiO3(001) surface remains unaffected by repeated cycles of adsorption-desorption, unlike other studies on ferroelectric surfaces [6,7].

References:

[1] K. Garrity, A.M. Kolpak, S. Ismail-Beigi, E.I. Altman, Adv. Mater. 22 (2010) 2969–2973 .
[2] A. Kakekhani, S. Ismail-Beigi, ACS Catal. 5 (2015) 4537–4545.
[3] A. Kakekhani, S. Ismail-Beigi, E.I. Altman, Surf. Sci. 650 (2016) 302–316.
[4] C.M. Teodorescu, J.M. Esteva, R.C. Karnatak, A. El Afif, Nucl. Instrum. Meth. Phys. Res. A 345 (1994) 141–147.
[5] K. Sakayori, Y. Matsui, H. Abe, E. Nakamura, M. Kenmoku, T. Hara, D. Ishikawa, A. Kokubu, K. Hirota, T. Ikeda, Jap. J. Appl. Phys. 34 (1995) 5443–5445.
[6] L.C. Tanase, N.G. Apostol, L.E. Abramiuc, C.A. Tache, L. Hrib, L. Trupina, L. Pintilie, C.M. Teodorescu, Sci. Rep. 6 (2016) 35301.
[7] N.G. Apostol, M.A. Husanu, D. Lizzit, I.A. Hristea, C.F. Chirila, L. Trupina, C.M. Teodorescu, Catal. Today 366 (2021) 141–154.

POSTER PRESENTATION

S2-PP4

Obtaining and tailoring electrical properties of epitaxial PZT thin films by different doping

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The outcomes of our experiments on ABO_3-structured epitaxial ferroelectric thin films are detailed here. Epitaxial thin films offer advantages in terms of controlled growth and strain engineering, which increases their ability to be tailored for specific applications. Materials that are ferroelectric show spontaneous polarization that can be induced by several factors, such as light, temperature, mechanical stress, and an electric field. These materials can play a significant role in various electronic and sensing applications or energy storage. Here, the research has focused on developing electrostatic solid-state capacitors from electrically polarizable materials such as $PbZrTiO_3$ (PZT) by finding a way to tailor their properties through doping or multilayering. The most typical characteristic of such materials is the significant nonlinear relationship between polarization (P) and applied electrical field (E), which is defined as the P-E loop. In order to obtain this, conductive oxides such as $SrRuO_3$ (SRO) or $LaSrMnO_3$ (LSMO) were grown as bottom electrodes for all structures that were grown on monocrystalline $SrTiO_3$ (001) substrates. The epitaxial relationship between the films and the substrate was analyzed by high-resolution X-ray diffraction (HR-XRD) and high-resolution transmission electron microscopy (TEM). The dependence of polarization orientation on the doping element was evidenced by piezoelectric force microscopy (PFM). The electrical characterizations of the epitaxial layers with different thicknesses were performed on capacitor-like geometry. This was achieved by top electrode deposition, SRO/Au or Pt by PLD, and magnetron sputtering using a shadow mask and defining ferroelectric capacitors of 100 μm^2 area. The obtained results show that doping influence the polarization orientation in the as-grown layer, which is associated with a change in conduction (n-type or p-type). We also found that by using doped PZT materials to design multilayers with different configurations, we are able to tailor the electrical properties to and make them suitable in different domains, such as non-volatile memories, field-effect transistors, or energy storage.

POSTER PRESENTATION

S2-PP5

The effect of magnetoelastic anisotropy on the magnetization processes in amorphous nanowires

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In this work, we report the theoretical and experimental investigation of amorphous glass-coated nanowires in order to understand the interplay between magnetoelastic and shape anisotropies. The hysteresis curves, the dependence of the switching field values on nanowire dimensions, and the effect of the magnetoelastic anisotropy on the magnetization processes were analyzed and interpreted to explain the magnetization reversal in highly magnetostrictive amorphous nanowires prepared in cylindrical shape by rapid quenching from the melt. Generally, we have several factors which influence the magnetic behavior in amorphous nanowires obtained by melt spinning: the direction of the applied field with respect to the easy axis, the anisotropy (magnetostatic and magnetoelastic contributions), and the dimensions of the nanowires (length and diameter). All the measured samples were found to be magnetically bistable, being characterized by rectangular hysteresis loops. We are modelling the hysteresis loops of the nanowires in the quasi-static regime using MuMax3 program [1] in which the magnetization process is fully controlled by the domain nucleation. The most important feature of the study is the inclusion of the magnetoelastic anisotropy term that originates in the specific production process of these amorphous nanowires [2]. The results show that the switching field decreases when the nanowire diameter increases and this effect is due to the reduction in anisotropy and in the intrinsic mechanical stresses. Moreover, the obtained results reveal the importance of factors such as geometry and magnetoelastic anisotropy for the experimental design of cylindrical amorphous nanowires for multiple applications in miniaturized devices, like micro and nanosensors.

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References:

[1] A. Vasteenkiste, J. Leliaert, M. Dvornik, et al., AIP Advances 4 (2014) 107133.
[2] C. Rotarescu, S. Corodeanu, C. Hlenschi, G. Stoian, H. Chiriac, N. Lupu, T.-A. Óvári, Materials 17 (2024) 1141.

POSTER PRESENTATION

S2-PP6

Structural and electronic properties of HfO_2 thin layers deposited on III-V semiconductor surfaces

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High k dielectric/III-V semiconductor interfaces are the most suitable alternative to the SiO2/Si tandem in the CMOS technology due to intrinsic material properties that bring unparalleled performance in the operation of electronic devices of new generation.

We report the obtaining of very thin films of HfO_2 on GaAs and GaSb semiconductor substrates by oxide-Molecular Beam Epitaxy (MBE) and Magnetron Sputtering deposition techniques. Stoichiometric semiconductor surfaces were obtained by combining wet chemical etchings (HF-H_2O_2-H_2O, H_2SO_4-H_2O_2-H_2O, HCl-H_2O_2-H_2O, $NaOH$-H_2O_2-H_2O solutions) with Ar ion etchings or thermal desorption in ultrahigh vacuum [1]. Deposition of very thin layers of 2nm and up to 40nm was carried out by MBE and Magnetron Sputtering techniques. Using XPS and ARXPS methods, the chemical structure of interfaces is revealed, proving a very abrupt interface of HfO_2/III-V semiconductor with traces of Ga_2O_3. No chemical reaction was observed between the HfO_2 and component elements of the substrate. Based on the Kraut method and implementing the REELS technique (Reflection electron energy loss spectroscopy), the energy band diagram of the interface is investigated, showing the position of the Fermi level at 0.64 eV from the maximum edge of valence band and band offsets of ΔE_C=1.7 eV and ΔE_B=2.4 eV respectively [2,3]. A band gap of 5.7-5.9 eV is found for the HfO2.

Measurements by Atomic Force Microscopy, X-ray Diffraction, and X-ray reflectivity provided data about the morphology of the layers, indicating a smooth growth without an increase in top surface roughness. The electrical measurements (I-V, C-V, G-V) were performed on MOS type capacitors using more metals as gate electrodes (Au, Ag, Al) and Au-Ge ohmic contacts on the semiconductor substrate. The HfO_2 layers show a dielectric value (k) in the range of 23-25 and usual values for the density of states at the interface (Dit ~ 10^{13} $cm^{-2}eV^{-1}$).

References:

[1] A.R. Clawson, Materials Science and Engineering R 31 (2001) 1–438.
[2] E.A. Kraut, R.W. Grant, J. R. Waldrop, S.P. Kowalczyk, Physical Review Letters 44 (1980) 1620–1623.
[3] T. Gouder, R. Eloirdi, R. L. Martin, M. Osipenko, M. Giovannini, R. Caciuffo, Physical Review Research 1 (2019) 033005.

POSTER PRESENTATION

S2-PP7

Hydrogenated GeSn films for short-wave infrared detection

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The hydrogenated Ge$_{1-x}$Sn$_x$ alloy is a promising material for the fabrication of photodetectors with sensitivity extended in the short-wave infrared (SWIR) further than 2 µm. By alloying Ge with Sn a transition from indirect to direct bandgap semiconductor occurs at Sn concentrations higher than 6%, increasing the optical transition probability. The main difficulty in obtaining this material is the low miscibility of Ge and Sn less the 1% Sn. However, high quality GeSn films up to 14 – 20 %Sn have been reported especially by epitaxial CVD growth, and thus laser emission could be obtained for the first time in direct bandgap group IV semiconductors. Amorphous and polycrystalline GeSn films with high Sn content can be easily obtained by versatile deposition techniques like magnetron sputtering (MS), but these films contain high density of structural defects generating deep level states that drastically affect the photosensitivity response. The hydrogenation during deposition can be employed to improve the photoelectrical properties of such GeSn films by healing structural defects, effect used since many years in fabrication of solar cells based on classical amorphous and micro-structured a-Si:H and a-SiGe:H hydrogenated semiconductors.

In this paper, we discuss the fabrication of Ge$_{1-x}$Sn$_x$:H thin films and their photoelectric properties. Ge$_{1-x}$Sn$_x$:H films that are deposited on GeSn by RF magnetron sputtering (MS) of Ge and Sn from separate targets. The hydrogenation of Ge$_{1-x}$Sn$_x$ was accomplished during deposition by adding either 10% or 30% hydrogen into Ar working gas. Amorphous Ge$_{1-x}$Sn$_x$:H films were obtained by MS deposition on c-Si and fused quartz substrates at room temperature, while dynamic nanocrystallization occurs by heating the substrates at 200 °C. Fourier-transform infrared spectroscopy transmission and reflectance measurements indicate higher hydrogen incorporation for low-temperature deposition and demonstrate the effect of hydrogenation on the absorption band gap. The structure and the formation of GeSn nanocrystals, as well as the Sn concentration have been investigated by using HRTEM micro-Raman measurements. The spectral distribution of the photocurrent and dark current were measured at different temperatures and bias voltages, showing a spectral photosensitivity extended to 2.2 µm. The hydrogenation increases the SWIR photosensitivity for a-Ge$_{1-x}$Sn$_x$:H amorphous films deposited at room temperature, in comparison to the nanocrystallized ones deposited at 200 °C which have lower incorporated hydrogen.

POSTER PRESENTATION

S2-PP8

Exchange bias effect in $ZnFe_2O_4$ (FIM)-FeO(AFM)-ZnO and ZnFeO (DMS) – FeO(AFM) nanocomposite systems

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Exchange-biased nanostructures represent an essential part of spin-based electronic devices. Examples of exchange bias effect applications are the magnetic tunnel junctions and spin valves used for magnetic sensors and computer/magnetic storage. In this context, the exchange biasing of dilute magnetic semiconductors, DMS, presents an important challenge. Our recent studies on Zn-Fe-O nanostructures produced by changing the Zn:Fe ratio (from 0.999:0.001 to 0.4:0.6 in at.%) in Zn(II)-Fe(III)-carboxylates (derived from acetate precursors) reveal that, depending on the nominal iron concentration and especially on the processing conditions, the following systems can be obtained: (i) Zn1-xFexO nanoparticles of the ZnO wurtzite structure (without any residual phases) showing weak room-temperature ferromagnetism, RTFM, characteristic of DMS, for iron concentrations below 3 at.% [1]; (ii) ZnO-$ZnFe_2O_4$ nanocomposites with $ZnFe_2O_4$ spinel of high inversion degree showing superparamagnetic (SPM) behavior at room-temperature for high iron concentrations, x equal to or higher than 0.03 [2]; (iii) Fe(FM)-FeO(AFM)-ZnO nanocomposites for x equal to or higher than 0.03 which exhibit the exchange bias effect, EB, [3] ascribed to the exchange coupling between the FM and AFM spins at the Fe/FeO interfaces after field-cooling from above the Neel temperature, TN, of FeO and below the Curie temperature of Fe. In the present presentation, we demonstrate that two other nanocomposite systems (less/or not reported in the literature) can be produced by controlling the processing conditions: (1) ZnFeO-DMS/FeO and (2) $ZnFe_2O_4$-FeO-ZnO. Both systems (1) and (2) show the EB effect (like system (iii)) despite the different constituents involved: a hysteresis loop shift, an improved coercivity of the ferromagnetic/ferrimagnetic phase and training effect. XRD, XPS, FTIR, Mossbauer and magnetization investigations indicates that: the EB in the system (1) might be related to the exchange coupling between the AFM and FM spins at the interfaces of FeO and ZnFeO-DMS nanostructures after field cooling from above the TN of FeO and below TC (higher than 300 K) of ZnFeO-DMS; EB in the system (2) can originate primarily from the exchange coupling between the FIM and AFM spins at the $ZnFe_2O_4$/FeO interfaces after field-cooling from above the TN of FeO and below the blocking temperature of $ZnFe_2O_4$.

References:

[1] V. Mihalache, C.C. Negrila, M. Secu, I. Mercioniu, N. Iacob, C. Kuncser, Results in Physics 51 (2023) 106644.
[2] V. Mihalache, C.C. Negrila, I. Mercioniu, N. Iacob, V. Kuncser, Phys. Chem. Chem. Phys. 23 (2021) 16107–16127.
[3] V. Mihalache, Results in Physics 58 (2024) 107469.

POSTER PRESENTATION

S2-PP9

Improvement of the tunnel magnetoresistance – based sensor by optimizing the deposition conditions

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In this work, we focused on improving the performance of tunnel magnetoresistance (TMR)–based sensors by optimizing the deposition parameters of the magnetic tunnel junction (MTJ) structure. Among magnetoresistive devices, MTJ structures exhibit higher magnetoresistance at room temperature [1], which makes them good candidates for a wide range of applications [2,3]. High-performance sensors based on the tunnel magnetoresistance effect must have a defect-free and smooth MgO barrier layer - the biggest challenge in the fabrication process.

For our purpose the MgO layer was obtained by electron beam evaporation, and all other component layers of the MTJ structure were deposited by magnetron sputtering on Si/SiO_2 wafers as follows: Ta(5 nm)/Ru(20 nm)/Ta(5 nm)/CoFe(2.5 nm)/IrMn(20 nm)/CoFe(2.5 nm)/Ru(0.85 nm)/CoFeB(3 nm)/MgO(1.8 nm)/CoFeB(3 nm)/Ta(10 nm). Atomic force microscopy (AFM) and scanning electron microscopy (SEM) were used to investigate the effects of the deposition parameters on the surface roughness of the individual thin film within the MTJ structure.

To verify the effect of the optimized deposition conditions on the performance of the magnetoresistive structure, TMR sensors were microfabricated in the CPP (current-perpendicular-to-plane) configuration and the variation of the electrical resistance was measured as a function of the applied magnetic field.

Through systematic analysis and optimization of the deposition parameters, the study shows a significant improvement in the tunnel magnetoresistance of the sensor from 49% to 60%, highlighting the importance of precise control of thin film properties for improving device performance.

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References:

[1] Y. Nagamine, H. Maehara, K. Tsunekawa, Appl. Phys. Lett. 89 (2006) 162507.
[2] N. Maciel, E. Marques, L. Naviner, Sensors 20 (2020) 121.
[3] Z. Q. Lei, L. Li, G. J. Li, C. W. Leung, J. Appl. Phys. 111 (2012) 07E505.

POSTER PRESENTATION

S2-PP10

Step meandering on vicinal surfaces: Crystal growth modeling based on cellular automata

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Self-organized surface morphologies resulting from various kinds of crystal growth processes remain a subject of large scientific interest through the years. Pattern formation of well-defined and ordered crystal structures is essential for technological evolution. Vicinal crystal surfaces can exhibit a number of different morphological instabilities, including the most widespread step bunching and step meandering, which appear as suitable templates for the growth of various nanostructures playing an important role in device manufacturing.

In the present study, we are focused on the step meandering instability obtained in the presence or absence of Ehrlich-Schwoebel barrier acting as an additional diffusion barrier at the step edges. We develop a two-dimensional atomistic scale model of vicinal surface growth based on cellular automata and combined with Monte Carlo diffusion. Recently introduced into our research, the cellular automaton appears to be a very useful tool in modeling and investigation of the process of pattern formation of growing crystals. Using numerical simulations of the proposed model, we explore how the surface evolution depends on various parameters such as height of Ehrlich-Schwoebel barrier, potential depth, adatom diffusion rate, initial adatom concentration and initial vicinal distance. The resulting surface morphologies show the emergence of step meandering which further evolves into regular finger-like structure of meanders. The presented analysis of the height-height correlation function allows for quantitative description of the surface morphology by extracting the proper characteristic length scales such as wavelength of meanders and amplitude of fingers. It is demonstrated that for a regular, well-ordered structure the correlation function calculated in direction along steps has an oscillating behavior which repeats regularly at a distance equal to the meander wavelength (*i.e.*, the correlation length). Therefore, the oscillation period can be properly related to the meander wavelength (or finger width), whereas the oscillation amplitude corresponds to the finger height. Using these characteristic lengths, we analyze the evolution of step meandering during the crystal growth process. For all studied cases at different parameters, the wavelength of meanders grows in time to its final value and we show how this value scales with various parameters. The time scaling exponents describing the growth of the characteristic length scales of pattern formation are also obtained. This study allows establishing the proper growth conditions to obtain surface patterns with regular step meandered structure that may serve as appropriate templates for nanotechnology.

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POSTER PRESENTATION

S2-PP11

Synthesis and characterization of kesterite thin films Cu2ZnSnS4 solar cells with Ag substitution

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Kesterite semiconductors, Cu_2ZnSnS_4 (CZTS), have been identified as one of the promising photovoltaic (PV) materials owing to their abundant elemental composition, wide band gap, high light absorption coefficient and non-toxicity. However, the significant open-circuit voltage deficit (Voc, def), linked among other things to the Cu-Zn disorder, is a critical limitation to the performance of Cu_2ZnSnS_4 solar cells. One strategy to mitigate this limitation is to make cationic substitutions in the CZTS crystal phase.

This study aims to improve the efficiency of kesterite solar cells through cation substitution, particularly by doping silver (Ag) into Cu_2ZnSnS_4 (CZTS) thin films to form $(Ag,Cu)_2ZnSnS_4$ (ACZTS) thin films. The study investigates the influence of various Ag concentrations on the band gap of ACZTS and capability to reduce antisite defects and disorder.

The ACZTS thin films were fabricated using spin-coating and sulfurization methods.

Stable solutions containing all the necessary cations and anions in the required quantities were produced. The precursor solutions were spin-coated onto a glass substrate coated with 20 nm of SiO_2.

The spin-coating steps were iterated from 1 to 5 times to reach the final desired thickness. Then, ACZTS thin films were heating (520 °C, 15 min) in a quartz tube containing sulfur powder and under a nitrogen N_2 flow to prevent oxidation of the layers.

Finally, the structural morphology and optical properties of the ACZTS thin films were analyzed using characterization techniques including X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and UV-Visible spectroscopy.

POSTER PRESENTATION

S2-PP12

3D-printed microfluidic devices for magnetic nano and microparticle synthesis of use in environmental applications

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Environmental applications of magnetic micro and nanomaterials are linked to actively researched scientific areas, with significant results in water/air decontamination, environmental-friendly applications, POP's level mitigation in protected areas, catalytic/photocatalytic removal of water contaminants, and many other high-end technical solutions in green chemistry. 3D printing technology offers flexible fabrication alternatives in 2D/3D microfluidic configurations related to costs, production times, material characteristics (*e.g.*, solvent compatibility, mechanical strength, temperature stress behavior, stability in aggressive chemical environments), and technical accessibility at the laboratory level. The present research is focused on developing new different microfluidic configurations with significant advantages, such as adaptive microfluidic liquid flow pathways, phase contact, proper reaction control, and tunable micro/nanomaterial morphology and properties. Two different nanomaterials were obtained: core-shell Fe_3O_4 nanoparticles and magnetic aerogel composites. The aerogel composites were obtained by final supercritical CO_2 desolvation, proving high surface areas, low densities, and tunable properties through surface functionalization (propyl-amino and non-polar surface grafting were performed). The primary applicability target of the obtained material was related to POP's removal/mitigation from aqueous environments, using the magnetic properties as a base for the final magnetic separation from the samples after POP's loading. The obtained materials and POP's extraction capacity were tested by advanced analytical methods: XRD, FT-IR, HR-MS, FT-ICR, Raman, SEM, TEM, and BET.

POSTER PRESENTATION

S2-PP13

Cross-flow 3D microfluidic device for aerogel nanocomposites synthesis

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Cross-flow 2D microfluidic geometries are well-known as efficient technical solutions in nanoparticle and nanocomposite materials synthesis. Most devices use 2D microchannels operated at low solvent flow rates with significant disadvantages related to productivity and geometrical restrainments. The present work proposes 3D multilayered geometries with highly configurable flow paths and the important advantage of high workflow operation capability. Tunability of nanoparticle/nanocomposite morphology can be obtained in correlation with reagents concentration range and flow rate adjustment. The proposed geometry uses 2x7 low-volume reaction chambers based on cross-contact of the involved reagents/precursors and a tangential high-level flow. The microfluidic device was assembled using in-lab processed PET sheets obtained by laser cutting and further mounted in the microfluidic assembly involving reagents, pumps, valves, and control devices. Operational testing stages were performed using in-lab developed protocols for aerogel nanocomposites comprising silica/alginate magnetic (Fe_3O_4) NPs. After supercritical CO_2 desolvation, advanced characterization methods were used (e.g., XRD, FT-IR, HR-MS, FT-ICR, Raman, SEM, TEM, and BET), in order to sustain the theoretical assumptions. The obtained 3D microfluidic device proves the expected flexibility related to nanocomposite size range, good reproducibility, and high production yield.

POSTER PRESENTATION

S2-PP14

Growth graphene by chemical vapor deposition for electronic devices

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Graphene is a two-dimensional (2D) material, which plays an important role in biosensors applications [1]. Chemical vapor deposition was employed to grow double- and multi-layer graphene on copper substrates and transferred to various substrates by electrochemical delamination. SEM analysis demonstrated the presence of a uniform, continuous graphene layer, while Raman Spectroscopy was employed to determine the number of graphene layers and the concentration of defects [2]. Electrical measurements showed a higher sheet resistance for double-layer graphene compared to multi-layer graphene. Also, physico-chemical characterization showed several differences between the two types of graphene, one set being related to structural properties including the number of layers and the concentration of defects, while a second being related to electrical conductivity. Further, the graphene was used as transducer for development of an electrochemical immunosensor for prostate-specific antigen (PSA) detection using anti-PSA as biorecognition element. Thus, the surface of graphene on a gold substrate (G/Au) was activated with EDC/NHS and functionalized with anti-PSA via 3-aminophenyl boronic acid. The detection of PSA was achieved by means of electrochemical impedance spectroscopy.

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References:

[1] L. Xu, Y. Wen, S. Pandit, V.R.S.S. Mokkapati, I. Mijakovic, Y. Li, M. Ding, S. Ren, W. Li, G. Liu, BMC Chem. 13 (2019) 112.
[2] I. Boukhoubza, M. Achehboune, I. Derkaoui, M.M. Apostol, M.A. Basyooni, M. Khenfouch, L. Nedelcu, I. Enculescu, E. Matei, J. Alloys Compd. 976 (2024) 173109.

POSTER PRESENTATION

S2-PP15

Dependence of La-doped ZnO nanocomposite properties of dopant concentration for semiconductor materials fabricated by electrospinning calcination method

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Zinc oxide is one of the most important types of metal oxides that have been studied thus far, due to its excellent properties such as high transparency, high exciton binding energy (60 meV) and low toxicity. It has been employed in various applications, such as gas sensors photovoltaic cells, fuel cells and even transistor fabrications. However, zinc oxide suffers from two main obstacles that limit its use. First, its high energy gap, which limits its absorption of visible light, limiting its uses in solar energy applications. Second its low electrical conductivity, which limits its uses in areas such as electronics and supercapacitors. One of the successful strategies for solving these two impasses is the doping process. Therefore, the effect of various metal dopants on the physical properties of zinc oxide was extensively explored. La-doped ZnO nanofibers were successfully synthesized by electrospinning, followed by calcination at 700 °C in air varying the dopant concentration from 0 to 5%. The microstructure and morphology of the La-doped ZnO nanocomposite semiconductors were evaluated by scanning electron microscopy (SEM), X-ray diffraction (XRD), and Raman spectroscopy. The characterization shows that the resulting La-doped ZnO semiconductors have a nanostructured tridimensional microstructure that is strongly affected by La dopant content. XRD characterization shows the presence of some La2ZnOx phase at higher concentration (e.g., 1%). SEM studies shows that increase of La concentration leads to an increase of nanocrystallites size (while XRD analysis shows that almost constant) and a radical change of shape and assembling of agglomerations into the 3D microstructures. The present results analysis lead reveal that by electrospinning-calcination used technique one can still obtain novel and interesting ZnO based nanocomposite semiconductors with unique properties.

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POSTER PRESENTATION

S2-PP16

Investigations of attograms and zeptograms of matter under extremely high electric fields

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Investigations on attograms and zeptograms of matter (1 attograms = 1e^{-18} gram, 1 zeptogram = 1e^{-21} gram) offer the possibility of exploring the transition between nanoscience and physics of molecules, opening the door for fundamental questions in soft-matter physics, such as for instance "What is the minimum amount of matter necessary to "define" the material properties?". Here we report an experimental approach that allows one, for the first time, to investigate zeptograms of matter under the influence of extremely high electric fields. Based on the concept of employing nanocontainers as experimental cells, our approach employs dielectric measurements by Broadband Dielectric Spectroscopy, to investigate, in a broad frequency and temperature range, the phase transitions of attograms and zeptograms of matter. Our approach opens the unprecedented possibility of carrying-out investigations at this small scale under extremely high fields (i.e. 1E^{5} V/cm) using low voltages (i.e. 4 V). We report the discovery of a zeptogram-effect that does not appear at the scale of attograms or above: the crystallization process in zeptograms partitions of ionic liquids can be reversibly switched off and on. This finding brings evidence for the ability of manipulating the state of matter, which opens the perspective of inducing new material properties different from those in the bulk or in nano-confinement.

References:

[1] A. Houachtia, G. Boiteux, G. Seytre, J.-F. Gérard, A. Serghei, Dielectric measurements on attograms and zeptograms of matter, Dielectric Newsletter 2016.
[2] A. Houachtia, P. Alcouffe, G. Boiteux, G. Seytre, J.-F. Gerard, A. Serghei, Nano Letters 7 (2015) 4311–4316.
[3] A. Serghei, W. Zhao, D. Miranda, T.P. Russell, Nano Letters 2 (2013) 577–580.

POSTER PRESENTATION

S2-PP17

X-ray diffraction and Raman scattering of PbSe(S) thin films

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In recent years, scientific research devoted to the optical properties of narrow-bandgap semiconductors with colloidal quantum dots has been growing intensively. One of the main reasons for this is that group IV-VI narrow-bandgap semiconductors have a two-photon absorption feature in the near and mid-infrared region of the spectrum. Another reason is its successful application in optical devices with low financial cost [1]. From the conducted studies, it is concluded that it is possible to adjust the optoelectronic properties of lead chalcogenides (PbSe and PbS) by the following methods: thermal treatment, changing the relative concentration of the chalcogen components included in the composition, changing the diametrical dimensions of the controllable quantum dots (in the range of 8.1÷16.1 nm) as a result of the joint effect of the mentioned [2]. Other studies show that the control of nanoparticle sizes in the intervals of 1.32 ÷ 2.26 nm and 1.28–2.48 nm in PbS(PbSe) materials obtained by the hot injection method, depending on the technological mode, lays the background for purposeful control of structural, optical and electrical properties [3].

The purpose of the work is to analyze the changes in the structural properties of lead chalcogenides (PbSe and PbS) thin films obtained by chemical bath deposition and the mechanisms of their influence on Raman scattering. Structural properties of PbSe, PbS and $PbS_{0.5}Se_{0.5}$ thin films and mechanisms of combinational scattering of light from phonons were studied by X-ray diffraction and Raman spectroscopy methods. The results of X-ray diffraction show that the crystallite sizes found in the thin layers of the studied substances are in the order of nanometers and vary in the interval d~10.7 ÷ 30.8 nm. It was determined that the scattering bands of the $PbSe_{0.5}S_{0.5}$ sample with large nanoparticle sizes shift to the region of large wave numbers compared to the scattering bands observed in the region of low wave numbers.

References:

[1] D. Wawrzynczyk, J. Szeremeta, M. Samoc, M., Nyk, J. Phys. Chem. C 120 (2016) 21939–21945.
[2] J. Liu, J. Liu, W. Zhang, K. Li, C. Liu, J. Non-Cryst. Solids 604 (2023) 122156.
[3] E. M. El-Menyawy, G.M. Mahmoud, R.S. Ibrahim, F.S. Terra, H. El-Zahed, I.K. El Zawawi. J. Mater. Sci.–Mater. Electron. 27 (2016) 10070–10077.

POSTER PRESENTATION

S2-PP18

In_2O_3 and ZnO thin film paper transistors fabricated by pulsed electron beam deposition

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Thin film transistors on paper continuously gain interest for emerging applications, such as flexible displays and sensors for wearable and disposable devices, making paper a promising substrate for green electronics and the circular economy [1,2]. This work concerns In_2O_3 and ZnO self-assembled thin film transistors on paper, the paper substrate being also the gate dielectric, fabricated by pulsed electron beam deposition (PED) at room temperature. The self-assembled source–channel–drain structures were obtained in a single deposition process using 200 and 300 µm metal wires as obstacles in the path of the ablation plasma. These transistors exhibited a memory effect with two distinct states that we shall further call “on” and “off”, characterized by a negative, respectively positive threshold voltage [2].

The In_2O_3 transistors present a field-effect mobility of 20 cm^2/Vs in both “on” and “off” states, similar to the measured Hall effect mobility of In_2O_3 thin films on paper. In the “on” state, we determined a subthreshold swing S=0.33V/decade, and a threshold voltage Vth on =-3.2V, while in the “off” state we had a subthreshold swing S=0.48V/decade and a threshold voltage Vth on =+0.4V.

The ZnO transistors exhibit a field-effect mobility of about 25 cm^2/Vs in both states. For the “on” state, a threshold voltage (Vth on = −1.75 V) and subthreshold swing (S = 1.1 V/dec) were determined, while in the “off” state, Vth off = +1.8 V and S = 1.34 V/dec were obtained [3]. The ZnO transistors have a maximum drain current of 1.6 µA in the “off” state, and 11.5 µA in the “on” state, while the In_2O_3 with the same paper substrate and geometry exhibit much larger maximum drain currents of 200 µA in the “off” state and 1 mA in the “on” state.

The study conclusion is that while In_2O_3 paper transistors are suitable for applications necessitating higher currents and better performance (smaller subthreshold swing), the ZnO paper transistors are promising as components for flexible, disposable smart labels and other various green paper-based electronics grace to ZnO’s non-toxicity.

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References:

[1] S. Nandy, et al.; Adv Mater. Technol. 6 (2021) 2000994.
[2] F. Gherendi, et al., Semicond. Sci. Technol. 28 (2013) 085002.
[3] F. Gherendi, D. Dobrin, M. Nistor, Micromachines 15 (2024) 265.

POSTER PRESENTATION

S2-PP19

How far oxygen deficiency can be driven in indium oxide thin films grown by pulsed electron beam deposition?

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Indium oxide is a transparent n-type semiconductor that has attracted considerable research due to its physical properties and is used in various applications including solar cells, optoelectronic devices, gas sensors, etc. [1]. Transparent indium oxide films are deposited by various thin film growth methods but black indium oxide films have been obtained and investigated to a much lesser extent. Pulsed electron beam deposition (PED), as an alternative to the well-known pulsed laser deposition (PLD), is an ablation plasma deposition technique for the growth of thin films of complex composition. PED allows precise tuning of deposition parameters for fine control of oxide thin film composition, morphology and physical properties [2].

A comparative study of black and transparent indium oxide thin films, both obtained by PED, is presented and the differences in terms of composition, structure, electrical and optical properties are reported. These films were grown on Si and c-cut sapphire single crystal substrates at different deposition temperatures and under oxygen or argon background gases. A slight variation of gas pressure around 0.01 mbar, specific to PED [2], results in a wide range of electrical and optical properties, from black oxygen-deficient to stoichiometric and transparent indium oxide films. X-ray photoelectron spectroscopy measurements of undoped and Sn-doped indium oxide thin films were carried out. A comparison of the spectra of undoped and Sn-doped indium oxide thin films grown with different oxygen deficiencies is presented and discussed in relation to the mechanisms limiting the carrier concentration in these films. As a result of their high oxygen deficiency, black indium oxide thin films show enhanced absorption in the visible and near-infrared spectral range, enabling them to extend their range of applications from transparent electronics to solar absorbers and photocatalysis.

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References:

[1] A. Klein, A. Frebel, K. A. Creutz, B. Huang, Phys. Rev. Mater. 8 (2024) 044601.
[2] M. Nistor, F. Gherendi, D. Dobrin, J. Perrière, J. Appl. Phys. 132 (2022) 225705.

POSTER PRESENTATION

S2-PP20

Investigation of the electrospinning parameters on the manufacture of PVDF nanofibers

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Nanotechnology has tremendously impacted many different science and engineering disciplines, such as electronics, materials science, and polymer engineering. Nanofibers, due to their high surface area and porosity, find applications as filter medium, adsorption layers in protective clothing, etc. Electrospinning has been found to be a viable technique to produce nanofibers. Piezoelectric polymers are promising energy materials for wearable and implantable applications for replacing bulky batteries in small and flexible electronics. Electrospinning is a facile process for controlled nanofiber fabrication by tunning the polymer solution, electrospinning parameters, and environmental conditions.

Polyvinyl difluoride (PVDF) and its co-polymer emerge as great interest toward flexible and sustainable piezoelectric nanogenerator with higher piezoelectric coefficients. PVDF is widely used as compared to other polymers because of its affordability, non-reactiveness, and chemical stability along with enhanced electroactive properties like piezoelectricity, ferroelectricity, and pyroelectricity. It has five different phases α, β, γ, δ, and Ɛ, α is a nonpolar thermodynamically stable phase, whereas β is the highest polar phase that shows maximum dipole moment and contributes piezoelectricity in PVDF. In this work, we investigated the process of electrospinning PVDF that affect the β phase percentage of PVDF by modifying its nanostructures, in the form of nanofibers. For the development of enhanced piezoelectric nanofibers optimization of *(a)* solution properties, *(b)* electrospinning parameters as well as *(c)* environmental conditions play a vital role. Manufacturing PVDF nanofibers by electrospinning is the simplest and most efficient technique to produce flexible, lightweight, biocompatible, ultrafine nanofiber of various thicknesses, and shapes with good material properties and high β content, emerges as an interesting candidate for energy harvesting applications in wearable and implantable devices.

POSTER PRESENTATION

S2-PP21

Amyloid beta improved surfaces for development of biomedical applications

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Nanostructured and biocompatible materials play a pivotal role in medical applications due to their unique properties such as large surface area, high surface energy, spatial confinement, and not harmful to the human body. When fabricated from conductive materials, these can stimulate cell proliferation, differentiation and tissue functionalities by promoting the transmission of natural bioelectric signals or electrical stimulation to cells and tissues that are electrically isolated. Considering these properties, one of the biomedical applications of conductive nanostructured materials address to neuronal cells, mainly due to the complexity of the nervous system and inefficiency of conventional repair methods.

Our study tries to support this kind of applications through the development and fabrication of novel conductive and biocompatible nanostructures materials to be further used in application involving neuronal cells. Thus, several conductive solid and flexible surfaces were fabricated using different types of glass, an electrospun polymeric nanofibers-based mesh and magnetron sputtering method for gold deposition. Scanning electron microscopy and X-Ray diffraction techniques were employed for a selection of conductive nanostructured materials to be used in further studies on living cells. To increase the biocompatibility and cell adhesion of cells at the selected samples, their surfaces were modified with different high ordered structural biomolecules such as poly-Lysine, collagen or amyloid peptides. Using the fibroblast L929 and the neuroblastoma SH-SY5Y lines as cellular model, the MTS assay, fluorescence and scanning electron microscopy investigations it was demonstrated that the new developed nanostructured surfaces are favorite candidates to be integrated in complex devices for cellular electrostimulation.

POSTER PRESENTATIONS

S2-PP22

Synthesis of a highly sensitive NH_3 gas detection sensor through Co-doped ZnO thin-film using SILAR Technique

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Sensors for ammonia (NH_3) gas detection are crucial for a range of industrial and environmental monitoring applications due to the harmful effects of ammonia on human health and the ecosystem. In this study, we present the synthesis of a highly sensitive NH_3 gas detection sensor using zinc oxide (ZnO) thin films doped with cobalt at concentrations of 0, 4, and 6% and fabricated by the SILAR (Successive Ionic Layer Adsorption and Reaction) technique. The SILAR technique offers precise control over the thin-film deposition process, enabling the manufacture of uniform, well-defined sensor layers. The synthesized samples were analyzed to assess their structural, morphological, optical, and gas-sensing properties. X-ray diffraction (XRD) revealed a hexagonal Wurtzite structure, and the crystallite size decreased from 23.29 to 22.17 nm. Energy dispersive X-ray spectroscopy (EDX) and Fourier transform infrared spectroscopy (FTIR) confirmed the presence of cobalt. A scanning electron microscope (SEM) was used to analyze the morphological features and demonstrate the presence of a nanosheet structure. The optical band gap was determined using Tauc diagrams, and as cobalt doping increased, the gap increased from 3.22 to 2.93 eV. Furthermore, atomic force microscopy (AFM) was performed to assess the surface topography. AFM measurements showed that the roughness increased from 243 to 406 nm. The results show that the optimum detection temperature is 250 °C. The cross-sensitivity shows a pronounced affinity of the sensor doped with 6% Co towards NH3, compared with the sensor doped with 4%. The dynamic responses show excellent reproducibility, with a response proportional to the NH_3 concentration, reaching a linear correlation of 90% with a low response and recovery time at a concentration of 150 ppm.

These results show remarkable improvements in response time and low operating temperature compared with existing work in the literature.

POSTER PRESENTATION

S2-PP23

Density functional theory computational study of the superconducting properties of palladium hydride systems

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The research for new room-temperature superconducting materials has led to the study of transition metal hydrides as potential superconductor candidates at high pressures. One such promising example is given by palladium hydride (Pd-H), which can embed relatively large amounts of hydrogen in its metallic interstitial sites even at ambient pressure. Through the present work, we aimed at investigating a range of stoichiometries from the $Pd_{1-x}Cu_xH$ system using density functional theory (DFT) in order to theoretically determine their potential crystalline structure, as well as their potential superconducting properties. Already-published experimental data was used to validate our computed structural optimizations, while the all-electron full-potential linearised augmented-plane wave code ELK served to predict the critical temperatures (TC). In addition, we determined the phonon density of states for Pd-H systems using the SIESTA code, which is a method more appropriate for large supercells.

References:

[1] S.S. Setayandeh, C.J. Webb, E. MacA Gray, Prog. Solid State Chem. 60 (2020) 100285.
[2] R. Vocaturo, et al., Journal of Applied Physics 131 (2022) 033903.
[3] T. Kawae, Tatsuya, et al., J. Phys. Soc. Jpn. 89 (2020): 051004.

POSTER PRESENTATION

S2-PP24

Exploring the generation of metal nanoparticles through laser ablation in liquid media

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Metallic nanoparticles hold significant importance across diverse industrial sectors owing to their distinctive attributes, including a high surface area-to-volume ratio and remarkable catalytic prowess. Notably, in catalysis or photocatalysis, metallic nanoparticles serve as highly efficient catalysts, expediting crucial chemical reactions pivotal to industrial processes [1]. Furthermore, their superior conductivity and optical properties empower advancements in electronics, facilitating the creation of cutting-edge devices with enhanced functionality and reduced size [2]. Pulsed laser ablation (PLA) in liquid environments holds promise for the fabrication of various nanoparticles (NPs) and nanostructures (NS). Globally, there is a growing demand for the production of metal nanoparticles, such as gold, silver, and nickel, for the manufacturing of sensors, optical and magnetic devices and photolytic processes such as water splitting [3].

This study outlines the principle of nanoparticle synthesis using a series of solid targets (Nickel, Terfenol 0.6 and 0.7, TiO_2, silver) and presents various experimental results obtained. For the experiments, wavelengths of 1064, 532, and 355nm were used, with a pulse frequency of 10 Hz and an ablation time of 20 minutes, corresponding to 12.000 pulses. As liquid suspensions, ultrapure water, ultrapure water + 5 mlM NaCl, and ultrapure water + 10 mlM NaCl were used. From the DLS data, the analyzed samples showed standard deviations of sizes, on average ranging from 15 to 100 nm, indicating a narrow distribution of nanoparticles and excellent stability. From the zeta potential, it is observed that the analyzed particles have anionic or cationic character. From the data obtained through atomic force microscopy, nanoparticles with sizes ranging from 10–40 nm and a maximum height of 100 nm were identified. From the data obtained through SEM, uneven distributions of nanoparticles with sizes ranging from 7–170 nm can be observed.

References:

[1] N. Narayan, A. Meiyazhagan, R. Vajtai, Materials 12 (2019) 3602.
[2] I. Matsui, J. Chem. Eng. Jpn. 38 (2005) 536–546.
[3] S.B. Singh, Nanomaterials for water splitting: A greener spproach to generate hydrogen. In: Kharissova, O.V., Torres-Martínez, L.M., Kharisov, B.I. (Eds), Handbook of Nanomaterials and Nanocomposites for Energy and Environmental Applications. Springer, Cham.

POSTER PRESENTATION

S2-PP25

The influence of duty cycle on structural and optical properties of Tin Selenide thin films prepared by pulsed electrodeposition

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This study investigates the pulse electrodeposition of tin selenide (SnSe) onto ITO(111) substrates. Thin films of SnSe were co-electrodeposited from an aqueous solution containing tin (II) dichloride ($SnCl_2$), selenium dioxide (SeO_2) precursors, and ethylene diamine tetra-acetic acid (EDTA) complexing agent at a temperature of 50°C. The electrochemical behaviors and codeposition potentials of Sn, Se, and SnSe were investigated using cyclic voltammetry.
Furthermore, the study explores the influence of duty cycle on the structural, morphological, elemental composition, and optical properties of the SnSe electrodeposited films. Characterization techniques including X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDX), and UV–vis absorption spectroscopy were employed.
The results reveal distinct differences between samples electrodeposited using pulsed and continuous methods. Samples deposited via pulsed deposition exhibited granular structures, while continuous deposition resulted in a nanosheet structure. Additionally, the samples displayed good stoichiometry, with an energy gap (E_g) ranging between 1.4 and 1.1, which decreased with an increase in duty cycle.

POSTER PRESENTATION

S2-PP26

Studies regarding the optimization of the dispersion process of iron oxide nanoparticles synthesized by laser pyrolysis

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The laser pyrolysis technique was used in the synthesis of magnetic iron oxide nano-powders with ethanol vapors as sensitizer. This technique uses the energy coming from a CO_2 laser working in C.W at 9.25 microns wavelength which is transferred to the reactive precursors via the excited ethanol molecules, generating a rapid heating of the $Fe(CO)_5$ vapors in the presence of oxygen. The presence of acetone in the gas product mixture revealed the partial decomposition of ethanol that it comes with positive role in NPs functionalization. Most of these nanoparticles exhibited superparamagnetic behavior at room-temperature with saturation magnetization values up to 60 emu/g and a mean particle size less than 10 nm. The samples consist mostly in maghemite with a decreased carbon presence when compared with the experiments with ethene as sensitizer. On the particles surface, ethanol decomposition generated functional groups such as -OH that act as a supplementary hydrophilic agent in nanoparticle water-based suspension. We studied the best dispersion and stabilization parameters of these nanoparticles simple or using various polymers such as: Sodium carboxymethyl cellulose, chitosan and l-3,4-dihydroxyphenylalanine. In optimized deagglomeration process values of zeta size around 80 nm and more than +40 mV zeta-Potential values were obtained. We noticed that the polymer presence in nanoparticle suspension comes with a further stabilization in time and the agglomerates are around 100 – 350 nm depending on polymers and their concentration. DLS analyses revealed a great stability in time at 4.8 to 5.3 pH (less than 5% variation of zeta size value up to 1 week) when chitosan was used.

POSTER PRESENTATION

S2-PP27

Spectacular dispersibility of oxide nanoparticles synthesized by laser pyrolysis with isopropanol vapors as sensitizer

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Nanofluids and nanostructures based on magnetically structures crystalline nano-domains have gained considerable attention in various applications including high density magnetic information storage devices, drug delivery, catalysts in the pharmaceutical industry, contrast elements in diagnosis, hyperthermia treatment, and many more. The low dimensionality of nanomaterials leads to an unusually high ratio between the number of atoms on the surface layers compared to those in deep, volume layers, and this leads to significant physical-chemical changes.

This paper will focus on specific experimental conditions for obtaining iron and stannous oxide nanoparticles, and the effect of the experimental parameters on the final properties of the material, including its dispersion in different fluids. Both types of NPs were synthesized with the laser pyrolysis technique. This technique is based on the interaction between a focused laser beam (CO_2 laser in quasi continuum regime) and at least one gaseous species in the precursor mixture. Iron pentacarbonyl ($Fe(CO)_5$) and Tetramethyltin ($(CH_3)_4Sn$) were used as precursors for iron oxide and stannous oxide nanoparticles, respectively. While the most common sensitizer used is ethane (C_2H_4), a weaker sensitizer (such as isopropanol) can come with the advantage that after the laser-molecule interaction the energy transfer is lower. Therefore, the C content of iron oxide samples obtained by laser pyrolysis using isopropanol as a sensitizer is lower than when ethane is used. In the case of tin oxide NPs, synthesis with isopropanol as sensitizer has a positive influence in tin dioxide formation as opposed to tin monoxide.

The elemental and structural characterizations (EDX, TEM, XRD) confirmed the nature of the particles, and DLS analysis indicated excellent stability of the samples in distilled water. Further, a reference sample was tested regarding its stability in organic fluids. The results displayed extremely reduced NP agglomerations with exceptional stability, even after 20 h. Moreover, this protocol did not hinder the magnetic behavior of the NPs.

POSTER PRESENTATION

S2-PP28

Exciton-photon coupling in ZnO optical microcavities fabricated by pulse laser deposition

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ZnO is a promising material due to its high excitonic binding energy (60 meV) that make possible the strong coupling of excitons-polaritons at room temperature [1]. This study was centred on the optical characteristics of ZnO optical microcavities with metal-oxides Bragg reflectors grown by pulsed laser deposition (PLD) on different substrates. The objective of our work was to highlight signatures of strong exciton-photon coupling, hybrid light-matter quasiparticles [2] in ZnO-based heterostructures for applications in the field of integrated quantum sources at room temperature.

The samples were investigated using both angle-resolved reflectivity and photoluminescence measurements of ZnO heterostructures. A set-up for angle-resolved spectroscopy investigations was buid-up in order to measure and confirm the formation of polaritonic states and to provides valuable insights about the exciton-photon coupling, such as strength, anticrossing behaviour and the dispersion relation [3]. The photoluminescence was measured at room temperature using as excitation source the third harmonic of Nd:YAG pulsed laser with emission wavelength at 355 nm, pulse duration of 5 ps and 500 kHz repetition rate. The reflectance spectra were recorded from spectro-ellipsometry measurements at incidence angles from 5° to 45°. The PL data corelated with the reflectance spectra evidenced the excitonic emission, the strong coupling regime and the formation of optical microcavity polaritons in our samples, at room temperature.

Acknowledgements:

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References:

[1] T. Makino, et al., Semicond. Sci. Technol 20 (2005) S78.
[2] F. Medard, et al., J. Appl. Phys 108 (2010) 043508.
[3] S. Ghos, et al., Photonics Insights 1 (2022) R04.

POSTER PRESENTATION

S2-PP29

Design and characterization of integrated optics fabricated by two-photon polymerization

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This paper aims to describe the process of building integrated optics structures, covering all the steps involved: designing, fabrication, and characterization. Two-Photon Polymerization (TPP) was used as method for fabrication of optical waveguides, splitters, gratings and coupling micro-optics as components for futures integrated optics devices. Integrated optics have become increasingly attractive in recent years because its applications can be used in many areas such as quantum technology, communication technology, computing, and sensoring. The main advantage of this technology compared to bulk optics is that it can be integrated with electronics much easier and can set up the stage for much smaller devices. The building process starts from the design of the structure which must be mathematically described to be able to perfectly control the edges of the structure. After the structure is defined, it must be simulated using dedicated software. The characterization process consists of pumping light into the structure and measuring its parameters. We have started our work by implementing a Y splitter using our own geometry, starting from the work of [1]. The splitting geometry consists of 4 circles with different radii and a spline curve that handles the sharp region. The structure has been analysed using COMSOL Multiphysics beam envelope method [2]. Moreover, we have conducted a parametric simulation to evidence the energy splitting ratio as a function of the building circle ratio. Also, we have analysed the behaviour of the waveguides with different widths and heights. For testing the structures, we have implemented two different coupling mechanisms, grating coupling and butt coupling. We have constructed two different setups and an application that allows us to control the stages and to characterize laser spots. As results, we observed the modes propagating through the structure using the grating coupling mechanism. The mode-pattern could have also been observed in COMSOL Simulations. We then moved on to constructing a structure consisting of a Y splitter and a Mach-Zehnder interferometer, which can be used as an entropy source for a Quantum Random Number Generator. Integrated optics will play a leading role in the quantum revolution and the increase in computational speed in various areas such as communication networks.

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References:

[1] Z. Lin, W, Shi, Opt. Express 27 (2019) 14338–14343.
[2] COMSOL Multiphysics, "The Wave Optics User’s Guide".

POSTER PRESENTATION

S2-PP30

Effect of doping on the structural and optical properties of Co-doped ZnO thin films by electrodeposition method

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Zinc oxide (ZnO) is a semiconductor material in thin film form with interesting chemical and physical properties that place it among the most promising materials in various fields: such as photovoltaic energy recovery, optoelectronics, photoluminescence, and gas detectors. Cobalt-doped ZnO on FTO-coated glass substrates was synthesized electrochemically (electrodeposition method), and the results obtained from scanning electron microscopy (SEM), X-ray diffraction (XRD), and UV-Visible spectroscopy showed that the optical gap increases with the increase of the percentage of cobalt doping as well as the formation of a Wurtzite crystal structure of ZnO.

POSTER PRESENTATION

S2-PP31

Study of optical and structural properties of mixed halides (I, Cl) of methylammonium-lead perovskite by spin-coating method for photovoltaic application

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Over the past two decades, organic halide-based perovskites have attracted a great deal of interest due to their potential applications in optoelectronic devices.

We have studied the effect of halogen X in methylammonium lead halide ($MAPbX_3$), where X = (iodide or chloride) deposited by spin coating. The MAPbX3 films obtained were characterized by X-ray diffraction (XRD), UV-Visible spectroscopy and scanning electron microscopy (SEM) and photoluminescence.

XRD analysis shows characteristic peaks of $MAPbX_3$ corresponding to peaks (100) and (200).

This analysis also shows the crystalline nature of the films produced. SEM images also show the good crystallinity of the films produced.

UV-visible characterization showed that the iodine-based sample absorbed better and had a good band gap (E_g= 1.95 eV).

POSTER PRESENTATION

S2-PP32

Growth and functionality of Cu_2ZnSnS_4(CZTS) films: From nanoparticle ink to inorganic solar cells

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Nowadays, the research in the photovoltaic field aims to find and investigate cheap functional materials based on earth-abundant elements. The Cu_2ZnSnS_4 (CZTS) is the candidate who has been widely studied in the last decade as an absorbing layer for applications in thin-film photovoltaics. The as-fabricated CZTS powder by hot-injection method were used to obtain nanocrystal ink to deposit the films by spin-coating method followed by annealing in sulfur atmosphere. The thermal treatment increases the grain size and improves the crystallinity of the films. The films were investigated by various characterization techniques: X-ray diffraction, scanning electron microscopy, Raman spectroscopy. Solar cells have been manufactured and the photovoltaic parameters were determined by measuring the IV curves of the corresponding solar cells. The present study gives promising results for new direction in solar inorganic cells devices.

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POSTER PRESENTATION

S2-PP33

Growth and characterization of vanadium dioxide thin films prepared by reactive-RF sputtering

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Vanadium dioxide (VO_2) thin films have received a lot of interest due to their metal-insulator transition (MIT) near room temperature, making them promising candidates for various electronic and optoelectronic applications. In this study, single-phase VO_2 thin films were synthesized using radio frequency (RF) sputtering on a (0001)-oriented sapphire substrate. A detailed characterization of the synthesized VO_2 thin films was carried out using X-ray diffraction (XRD), Raman spectroscopy, Rutherford backscattering spectrometry (RBS), scanning electron microscopy (SEM), atomic force microscopy (AFM), and X-ray photoelectron spectroscopy (XPS). The XRD analysis of the VO2 thin films showed a high degree of texture, with the majority of the crystalline grains aligned in the [010] direction. The rocking curves of the (020) reflection demonstrated strong crystalline quality, with a full width at half-maximum of 0.13°. According to SEM and AFM measurements, the VO_2 thin films have a compact and uniform shape, and the early phases of thin film formation indicate the Volmer-Weber growth mode. The surface of the VO_2 thin films showed only the V^{4+} oxidation state, according to the XPS analysis. The elemental composition of the films was estimated through RBS, revealing a composition of $\{V, O\} = \{0.36, 0.64\}$. The electrical resistivity of the VO2 thin films was found to differ significantly by four orders of magnitude at the phase transition temperature of 339 K. This result is consistent with the previously reported values for monocrystalline VO_2 (341 K). All of this emphasizes the potential of the synthesized VO_2 thin films for electronic devices and sensors, among other applications that need precise control over electrical characteristics. Moreover, the ability to tailor growth conditions and control film properties opens avenues for further optimization and customization to meet specific application requirements.

POSTER PRESENTATION

S2-PP34

Polarization switching triggered by charge injection: possible universal switching mechanism in ferroelectric thin films

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Ferroelectrics are materials possessing spontaneous polarization that can be switched by the application of a suitable external electric field. Therefore, the polarization-electric field (or voltage) (P-E(or V)) dependence describes a hysteresis loop. The polarization switching is commonly described by nucleation and growth of ferroelectric domains. All the models based on domain formation neglect the last phase of the switching, consisting in redistribution of charges involved in the compensation of the depolarization field that it is present in the films immediately after switching. Here it is shown that in this phase the ferroelectric film with electrodes behaves more likely as a resistor, and it is suggested that the switching is triggered by the charge injection into the film, most probably without formation of ferroelectric domains. This model is based on the observation that, during the first phase of the switching, the increasing part of the current peak associated to polarization switching has a quasi-linear dependence on voltage, suggesting a resistive behavior, not a capacitive one. The resistance extracted from this parte has voltage, frequency, and a very weak temperature dependence that can be explained by assuming an ohmic like dependence of current density on the applied electric field. This can be obtained when the Schottky barriers at electrode interface become negligible and a massive charge injection is possible. The study was performed mainly on epitaxial $Pb(Zr,Ti)O_3$ films, but similar resistive like behavior during switching was observed also for $BaTiO_3$, $BiFeO_3$, Mn doped $BiFeO_3$, $Pb(Zr,Ti)O_3$ films with different top electrodes, and even for $Hf_{0.5}Zr_{0.5}O_3$ films. These results suggest that polarization switching triggered by charge injection might be a universal mechanism, at least in inorganic displacive like ferroelectrics.

POSTER PRESENTATION

S2-PP35

Exploring the structural and chemical composition of antimony monolayer on Ag(110)

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The unique characteristics of silicon nanowires have generated significant interest in developing comparable structures using alternative materials. Especially heavier elements such as Sn, Sb, or Bi are interesting materials due to their spin-orbit coupling, making them promising candidates for topological insulators. This study focuses on antimony, which has already been fabricated in a nanowire arrangement on Ag(111) [1].

However, the preparation on a (111) surface raises the question of whether the row-like arrangement of the Ag(110) surface is more suitable for the preparation of nanowires.

The electronic properties and structural arrangement of the adsorbate are highly dependent on the surface and interface structure of the system. Consequently in our study we focus on investigating the surface and interface of the Sb/Ag(110) system.

This study investigates the impact of layer-thickness and annealing temperature on the structural and chemical composition of the monolayer Sb-phases. Therefore we use surface sensitive methods, namely low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and scanning tunneling microscopy (STM). Our results show a dependence on both, temperature and layer-thickness, with different structural and chemical arrangements. The chemical composition of antimony monolayers on Ag(110) presented in this study has not been previously reported to our best knowledge. For different layer thicknesses, three chemically distinct phases were identified through XPS measurements, even though two of them appeared structurally identical in LEED with a c(2x2) reconstruction. Additionally, it was discovered that the XPS component to the c(2x2) structure is only weakly bound to the Ag substrate. While the first c(2x2) reconstruction was obtained for a coverage of 1/4ML, the second c(2x2) phase was identified as a transition phase to the third observed phase. The third phase was obtained at higher coverage with a distinct and quite complex structural arrangement in LEED. The results of the higher coverage phase are consistent with the discovery of Sb-nanostrips by Wang et al. [2].

Furthermore, this study follows up on our previously published results investigating low-dimensional germanium on Ag(110) [3].

References:

[1] S. Sun, T. Yang, Y.Z. Luo, et al., J. Phys. Chem. Lett. 11 (2020) 8976–8982.
[2] Y. Wang, Y. Song, W. Zhang, et al., J. Phys. Chem. C 126 (2022) 15030–15036.
[3] L. Kesper, M. Schmitz, C. Westphal, et al., Appl. Nanosci. 12 (2022) 2151–2160.

POSTER PRESENTATION

S2-PP36

2D-MoS$_2$ selectively grown on Mo patterned substrates for photosensitive field effect transistor

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Atomically thin films of MoS$_2$ were selectively grown on Mo patterned substrates for the formation of intimate metallic contact and easily fabrication of devices [1]. Mo-CVD growth method in which MoO$_2$ from oxidized Mo pads and S powder as growth precursors was employed. Mo thin film of 30 nm thickness was deposited by magnetron sputtering on SiO$_2$/Si substrates and patterned by photolithography to obtain Mo strips and finger contacts with gaps of 5 to 20 µm between Mo electrodes. 2D MoS$_2$ interconnected flaks of 1-2 monolayers filling the gap between Mo contacts were obtained, as shown by SEM and AFM imaging. Photo-FETs with 2D MoS2 selectively grown between source-drain Mo contacts and Si substrate used as gate one was fabricated for photoelectric characterization. By varying the gate voltage from +7 V to -7 V, the dark current is drastically reduced from 10-9 A to 10-13 - 10-14 A, showing the n-type semiconductor behavior of the selectively grown 2D MoS$_2$ film. High Iph/Idark photosensitivity of 105 (%) was obtained with Vsd of 0.5 V and Vg of -5 V, for 4.5x10-4 mW/cm2 of 650 nm monochromatic light. The spectral responsivity measured for the sensitive case of Vg = -7V reaches values of 15 – 25 A/W at 600 nm wavelength, and reveals the onset energy of 1.72 – 1.77 eV and A and B excitonic absorptions.

References:

[1] I. Stavarache, C. Palade, A. Slav, I. Dascalescu, A.M. Lepadatu, L. Trupina, E. Matei, M.L. Ciurea, T. Stoica, ACS Appl. Nano Mater. 7 (2024) 5051–5062.

POSTER PRESENTATION

S3-PP1

New deposition method for achieving ferroelectric orthorhombic ZrO_2

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Ferroelectric materials have shown great potential for applications in energy storage capacitors, memory devices, sensors, photodetectors, etc. In the case of memory devices, the discovery of ferroelectricity in Si doped HfO_2 in 2011 paves the way towards an extensive research about the possibility of achieving robust ferroelectric polarization in sub 10-nm thick HfO_2-based films. The existence of this surprising behavior was understood by the existence of a novel non-centrosymmetrical orthorhombic phase with space group Pca21 and the strong interest on these materials arises from their full compatibility with standard complementary metal oxide semiconductor (CMOS) processing.

In the present work, a new deposition method, nano-second laser annealing, of ZrO_2 thin film having as top and bottom electrode, W, is investigated in order to stabilize the ferroelectric orthorhombic crystalline structure. X-ray diffraction and transmission electron microscopy analysis were used to elucidate the formation of the orthorhombic phase of ZrO_2 together with minor monoclinic phase. As well as being advantageous for producing rapid crystallization, compared to standard annealing, which is based on RTA (rapid thermal annealing method), NLA can strongly reduce W oxidation as the annealing time is very short, in the ns range. Overall, we provide experimental evidence for the formation of the o-phase by combining TEM (transmission electron microscopy) analysis together with EBSD and XRD techniques, for the $Si/SiO_x/W/ZrO_2$ film stack and stable ferroelectric performance is obtained.

POSTER PRESENTATION

S3-PP2

Production of a few alpha pairs in interactions of light nuclei with nuclear emulsion

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Experiments with nuclear beams at energies of a few GeV are recognized as the most promising ways to understand the basic properties and intrinsic structure of nuclei. In these nuclear research experiments, as in the present one, the nuclear emulsion was the target and detector.

The technique of nuclear emulsions offers an overview in the field of relativistic nuclear physics due to the high accuracy of the events that can be observed, the excellent high spatial resolution (of order 0.5 microns), and the almost total observation of the tracks of charged particles as could be seen.

This paper presents the result obtained in Monte Carlo simulation for a few alpha pairs in final state from interactions of light nuclei with nuclear emulsion. Geant4 code was used in order to obtain MC data and the implemented geometry was similar to the BECQUEREL experiment. A parallel description of simulated data and experimental data will be shown.

POSTER PRESENTATION

S3-PP3

From electron tomography to magnetic properties using micromagnetic simulations

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Electron tomography is a nanoscale 3D technique that has become a standard in material science and engineering, but the extraction of quantitative information requires elaborate processing of the data.

Different methods of evaluating the magnetic shape anisotropy energy and the demagnetization factors of an ensemble of magnetic nanoparticles (MNP) via electron tomography are presented. An extension of a previous in-house developed software has been made [1]. This software was written for processing 3D data in order to retrieve quantitative morphological information regarding nanoparticle systems. The acquired data about the nanoparticle system, constitute input data to micromagnetic simulations programs which provide information about the magnetic properties of the studied system.

Iron oxide (magnetite) nanoparticle systems have been prepared using coprecipitation methods. The tomographic series was acquired using JEOL 2100 transmission electron microscope (TEM). Tomographic reconstruction was performed using GENFIRE [2] software. The quantitative information regarding the nanoparticle size and shape was obtained using the above-mentioned software. The relevant data is saved in a suitable format in order to be used by the Object Oriented Micro Magnetic Framework (OOMMF) [3]. Magnetic information is retrieved by numerical simulations and is compared with similar information approximated using only morphological information.

Morphological information (size, shape) corroborated with magnetic information (demagnetization factors, shape anisotropy energy) are relevant in fields like gas sensing [4], catalysis, spintronics and magnetic hyperthermia-based therapies [5].

References:

[1] C. Radu, et al., Beilstein J. Nanotechnol.13 (2022) 590–598.
[2] A. Pryor, et al., Sci Rep 7 (2017) 10409.
[3] M.J. Donahueand, D. G. Porter (1999), OOMMFUser'sGuideVersion1.0. (National Institute of Standards and Technology, Gaithersburg, MD,1999), http://math.nist.gov/oommf/.
[4] A. Stanoiu, et al., Chemosensors 9 (2021) 125.
[5] S. Tandon, et al., Journal of Magnetism and Magnetic Materials 271 (2004) 9–16.
[6] J. A. Osborn, Phys. Rev. 67 (1945) 351.

POSTER PRESENTATION

S3-PP4

Structural and photophysical properties of antimony hybrid perovskites for organic light emitting diode applications

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Halide perovskites are a class of materials that have recently emerged as a promising option for optoelectronics and photovoltaics applications. This is due to their unique characteristics such as high photoluminescence quantum yield, tunable emission wavelengths, and defect-tolerant properties. Additionally, these materials can be synthesized at room temperature without compromising their physical properties. The composition of halide perovskites is AMX3, where A is the organic cation (e.g. $NH_4{}^+$, $CH_3NH_3{}^+$), M is the metal cation (usually tin or lead), and X is the halogen anion (iodine, bromide, chloride). The organic-inorganic halide perovskites have a direct band gap which can be tuned from blue to infrared [1], making it suitable for optoelectronic devices. It also has a large absorption coefficient [2] and long electron/hole diffusion lengths [3], further increasing its potential use. Antimony perovskites, a type of halide perovskite, have also been found to be useful for applications in optoelectronics. These materials can form nanocrystals with an A3Sb2X9 configuration, with an optical band gap of 2.2 eV [4]. The nanocrystals comprise bi-octahedral anionic metal halide clusters surrounded by MA+ cations. To synthesize antimony perovskites, antimony halide and methylammonium halide are used as perovskite precursors using gamma-butyrolactone, dimethylformamide as polar aprotic solvents, and toluene anhydrous as an antisolvent. The structural and photophysical properties of antimony perovskites are currently being investigated to determine their potential use in OLEDs. With their unique characteristics, halide perovskites could have a significant impact on the future of optoelectronics.

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References:

[1]. H.S. Jung, N.G. Park, Small 11 (2015) 10.
[2]. S. De Wolfet, et al., J. Phys. Chem. Lett. 5 (2014) 1035.
[3]. S.D. Stranks, et al., Science 342 (2013) 341.
[4]. K.M. Boopathiet, et al., J. Mater. Chem. A 5 (2017) 20843–20850.

POSTER PRESENTATION

S3-PP5

Exploring underwater objects through magnetometry techniques - methods and assessment

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Magnetometry, a crucial asset in marine underwater exploration, provides excellent insight into methods of discovering and classifying submerged objects by offering effective tools for their characterization and mapping. From this perspective, the investigation of the terrestrial magnetic field emerges as a pertinent issue in understanding and interpreting anomalies generated by materials with ferromagnetic properties.

Utilizing magnetometry methods, the analysis of changes in the Earth`s magnetic field enables the detection of such materials on the surface. By closely examining the magnetic materials of submerged objects, a comprehensive assessment of their historical context, construction, and potential artefacts can be made.

Through analysis of magnetic field data, encompassing anomaly detection and interpretation, this paper presents a systematic approach to uncovering the mysteries concealed beneath the sea`s depths, by analyzing key elements of magnetic field theory and illustrating how magnetometry data collected along the Romanian coastline have been interpreted.

POSTER PRESENTATION

S3-PP6

Effects of several accelerators` working mechanisms on Portland cement concrete structure and mechanical properties

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The increasing demand for infrastructure, the necessity to rehabilitate old structures, and the changes in the global climate require the realization of new cement-based materials with lower setting times. As the most appropriate manufacturing additive, accelerators can meet these crucial requirements. In this novel study, new cement-based concretes were designed using the following accelerators: calcium nitrate, sodium thiosulfate, and aluminium sulfate individual and in several combinations. The effects of these accelerators on the structure and mechanical properties of early-stage Portland cement concrete at the 7th day curing time were studied using X-ray diffraction (XRD), Scanning Electron Microscopy with an Energy Dispersive Spectrometer (SEM-EDX), and measuring the compressive strength. The XRD Diffraction patterns of the investigated samples revealed the presence of crucial crystalline phases: quartz, portlandite, larnite, calcium silicate, ettringite, albite and muscovite. The semi-quantitative analysis of the samples showed a competition between quartz and muscovite as the main components of these concretes, while the content of C_2S and C_3S varies slightly. The SEM-EDX distinguishably showed the presence of portlandite and ettringite in concretes and allowed the measurement of holes and the distance between them. The chemical composition was obtained, and the ratios Ca/Si and Ca/(Si+Al) were calculated. The values of compressive strength range from 25 to 35N/mm2. The highest value for additive samples was obtained for concrete with added calcium nitrate. This study showed the impact of additives on the structure of regular concrete and is a step in elucidating their working mechanism while added to concrete.

POSTER PRESENTATION

S3-PP7

Scanning electron microscopy as pathway to study on the adherence of nanomaterials on cells

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When studying the interaction between cells and nanomaterials, it is essential to image the effects of the material on the cell membrane. High Resolution Scanning Electron Microscopy (HR-SEM) is an effective method for evaluating the results of this interaction process as opposed to just imaging them using a conventional inverted microscope. Magnetic particle-mediated cancer treatment can be achieved through magnetic hyperthermia or magneto-mechanical actuation. In order to know how these nanomaterials adhere to the cell surface, we need to obtain reliable images of their interaction, to determine if a sufficient quantity is on the cell surface, as well as their distribution on the cell membrane.

This protocol outlines a simplified and effective method for preparing cell-based biological samples to observe nanomaterial surface adherence using SEM. For this new protocol we used silicon wafers as a substrate to grow cells, followed by the addition of the evaluated nanomaterial to the cell culture media for at least 24 hours of incubation. Next, the samples were washed to remove any non-adhered nanomaterials, and then fixed with glutaraldehyde and osmium tetroxide. The silicon wafers were dehydrated using increasing concentrations of alcohol and air-dried in the biological safety hood and vacuum, followed by a coat with a 5 nm gold sputtered film. Finally, the samples were imaged using HR-SEM. For this purpose, we used different types of cells, i.e. normal dermal fibroblasts (NHDF), human osteosarcoma cells (HOS) and adipose-derived mesenchymal stem cells (ADSC) loaded with magnetite nanoparticles or Co-Fe nanowires. One of the advantages of using this new method is the replacement of difficult steps such as critical point drying of the samples to make the method quicker and easier to perform. Using SEM imaging we can estimate nanomaterial interaction with the cell surface. For example, MNPs are concentrated on the ADSC and NHDF cell membrane, but avoiding the area with the nucleus while for HOS the MNP are equally dispersed. For the observation of NWs, using HR-SEM, we can see that for some samples, the NWs can spear the cell membrane, phenomenon not visible on the inverted microscope, while for others, the NWs just adhere to the cell membrane surface without affecting them in any way.

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POSTER PRESENTATION

S3-PP8

Hydrogen isotopes released from beryllium layer by laser induced desorption and laser induced ablation

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One of the most extensive research subjects in the last decades is the thermonuclear fusion due to its great potential to provide an alternative energy source using as main fuel hydrogen isotopes (deuterium and tritium) [1]. An important issue, regarding the use of hydrogen isotopes is the easiness to penetrate the materials relevant for fusion technology [2]. Thereby, the study of incorporation, retention, and desorption of hydrogen isotopes from nuclear materials by mass spectrometry hold an important task in the nuclear fusion field [2].

The aim of this work is to study the release of deuterium atoms from 1 µm co-deposited deuterium-beryllium layer by laser induced desorption. The layer was obtained by combining the thermionic vacuum arc method with a deuterium plasma torch. A 1053 nm laser source, operating with 10 ns pulse duration and 1 kHz repetition rate, was used to achieve a high deuterium release and low surface damages. A dedicated home-made software control was developed for variation of laser pulse energy, laser repetition rate, in order to obtain the transition from ablation to desorption of deuterium-beryllium layer. The threshold between the ablation and desorption is attain when laser source delivers between 3 pulses where no BeO, BeD, and SiO species in optical emission spectra and mass spectra were measured. The amount of deuterium released from beryllium layers after laser irradiation was evaluated by quadrupole mass spectrometry. The results were compared with the one obtained by thermal desorption spectroscopy, which indicated a total amount of deuterium of about 4.04 × 1017 D at/m2. The results indicated that 100 % and 1.3 % of atoms were released after samples exposure to 400 laser pulses respectively 5 laser pulses. A discussion on the effects of the laser beam operating parameters on the layer's morphology is also presented.

The present work is the continuation of study from ref. [3] where the deuterium was released from aluminum layers.

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References:

[1] D. Cao, *et al.*, Analytical Methods 9 (2017) 3067–3072.
[2] B. Schweer, *et al.*, J. Nucl. Mater. 363–365 (2007) 1375–1379.
[3] S.-A Yehia-Alexe, *et al.*, Spectrochimica Acta Part B: Atomic Spectroscopy 208 (2023) 106774.

POSTER PRESENTATION

S4-PP1

Improving the conductivity of FETs based on carbon nanomaterials by decorating the nanomaterial surface with gold nanoparticles

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One of the methods to improve the conductivity of carbon nanomaterial-based field effect transistors is to decorate the surface of the carbon nanomaterial with various nanoparticles that could have a more efficient interaction with the underlying nanomaterial, thus creating higher conductivity. We used electrochemical methods to modify the electrical conductivity of the source-drain channel of FETs with gold nanoparticles, since one can control the nanoparticle morphology, size, and location. The electrochemical fabrication of gold nanoflowers involves the use of electrochemistry to induce the reduction of gold ions (Au^{3+}). The process was performed in a solution containing gold ions, 0.5 M H_2SO_4 in 2 mM $HAuCl_4$. The general steps of the process are *(i)* preparation of the gold solution, *(ii)* choice of the electrode, *(iii)* immersion of the working electrode in the solution containing gold ions, *(iv)* application of an electric potential between the working electrode and the reference electrode specific to the electrochemical cell in which the experiments are performed, *(v)* growth of gold nanoflowers (AuNFs), *(vi)* size and shape control: Through these steps, gold nanoflowers with controlled size and shape were obtained, which will be able to be used in a variety of applications, including biosensors, catalysts and other fields. Several electrochemical procedures have been developed for growing AuNFs in source-drain channels of vertical graphene and nanocrystalline graphite, and on glassy carbon, varying the potential range and scan rate. The results indicated an increase of the FET's conductivity up to 5 times, compared with the measurements before the AUNFs decoration.

POSTER PRESENTATION

S4-PP2

Advancements in smart material systems for micro 4D printing: fabrication, actuation and characterization

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Macro 4D printing has become a well-established technology within the medical domain, facilitating the creation of various devices like prosthetics, implants, splits, stents, pharmaceuticals and targeted drug delivery systems. This technology`s ability to craft intricate geometries with real time adaptability from the printing platform sets the stage for novel applications in soft robotics, self assembling structures and microscale photonics and optical devices (1). However, several significant challenges remain, including limitations in hardware and materials, constraints on mechanical properties of printed objects, slow and imprecise actuation and insufficient control over deformation phases (2). This study aims to propose and compare two smart material systems, specifically photoresists suitable for two photon polymerization (2PP) micro 3D printing.

In this investigation we demonstrate the fabrication and actuation of microstructures with sizes ranging from 10 to 100 micrometers, utilizing a pH-responsive hydrogel and a light-responsive liquid crystal elastomer (LCE). We produced these microstructures via 2PP micro 3D printing using a Nanoscribe Photonic Professional GT. We optimized the fabrication process by adjusting the exposure dose and structural parameters. Subsequently, we characterized the resulting structures in terms of topology and material response, mainly size changes upon actuation. We propose and discuss a model describing the impact of the fabrication parameters on material response and establish a set of fabrication parameters for producing microstructures with a good balance between two desired properties, mechanical stability and actuation.

Overall, our study confirms the feasibility of employing two distinct home-made photoresists for micro 4D printing and offers guidance on their processing. These materials hold promise for integration into innovative microtools that will shape the future.

References:

[1] Advanced Materials 35 (2023).
[2] Z. Zhang, et al., Journal of Smart and Nano Materials 10 (2019) 205–224.

POSTER PRESENTATION

S4-PP3

Study of protonated diamines for the improvement of the morpho-structural characteristics of hybrid halide perovskite films

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Sustainable energy production is one of the critical challenges that society needs to solve in the following years to sustain the progress towards a net zero carbon future. As part of the European REPowerEU strategy [1] to accelerate the deployment of renewable sources and replace fossil fuels, and in particular, to reduce dependence on imports from Russia, the European Commission has set solar capacity targets of 400 GW by 2025 and 740 GW by 2030.

In the last fifteen years, hybrid organic-inorganic halide perovskites have evolved into an increasingly significant challenge due to their tremendous potential as a light absorber material. Considering its special qualities and the low-cost potential of perovskite photovoltaic (PV) technology, perovskite solar technology is anticipated to overtake conventional solar technology both as single junction devices, as inexpensive perovskite panels and as tandem structures (multi-junction) with current silicon modules [2].

The main vulnerabilities of hybrid perovskites include surface and grain boundary trap site development, as well as their susceptibility to moisture. Some of the most promising additives or surface ligands for enhancing the performance of perovskite solar cells (PSCs) are amines that can be employed as spacers to generate a two-dimensional (2D) perovskite or as a capping layer due to their hydrophobicity.

Here, we present our work focused on the compositional engineering of the hybrid perovskites to improve the stability of the material. We present studies on three types of diamines, 1,4-diaminobutane (DMB), 1,6-diaminohexane (DMH) and 1,8-diaminooctane (DMO) and their influence on methylammonium lead halide hybrid perovskite films (MAPICl). All three must be protonated into a halide form to ease their integration as substitutes or additives in the perovskite precursor solutions. The modified perovskite films were morpho-structurally characterized and used as active films in solar cells.

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POSTER PRESENTATION

S4-PP4

Evaluation of the viability of 3D stem cell spheroids in a hydrogel matrix for dental tissue regeneration

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The method of DPSC cultivation was set up in agarose-coated microplates, in different conditions, using liquid overlay technique [2], to prepare several experimental variants of 3D spheroids. The morphology of 3D spheroids was observed by light microscopy and their structure by TEM. Cell viability was assessed by Live/Dead staining at 3 and 7 days of cultivation. The spheroids were cultivated in a natural polymeric hydrogel, in osteogenic culture medium, and the capacity to secrete extracellular matrix-specific constituents was investigated by ELISA techniques.

The results allowed optimization of a lab biotechnology and cell cultivation parameters to obtain 3D spheroids based on DPSC self-assembly capacity. Light microscopy observations revealed spheroids with spheric or ellipsoidal shape and controllable size (150-800 micrometers in diameter), according to initial cell density and period of cultivation. TEM analyses showed that DPSC spheroids consisted of an outer layer of viable fusiform cells with microvili, a middle layer of latent cells with condensed nuclei, and a necrotic core of disintegrated cells due to hypoxia and lack of nutrients. In addition, peripheral cells had dilated rough endoplasmic reticulum and were metabolically active. Live/Dead staining indicated that spheroids maintained high cell viability on the entire period of cultivation.

The results obtained on 3D spheroids-hydrogel system showed specific osteogenic markers synthesis. Thus, alkaline phosphatase secretion reached the highest level after 21 days of cultivation. The mineralization process was characterized by calcium secretion and nodule formation, while the procollagen production was constantly increasing.

In conclusion, all these results allowed selection of functional variants of DPSC spheroids secreting extracellular matrix and their cultivation in polymeric hydrogel demonstrated osteogenic properties, playing a role in further applications in periodontal tissue regeneration.

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This work was supported by the Ministry of Research, Innovation and Digitization, Program Nucleu, Project 23020201 and UEFISCDI, contract 62PCE.

References:
[1] C. Yun, et al., Int. J. Mol. Sci. 25 (2024) 2512.
[2] N.E. Ryu, et al., Cells 8 (2019) 1620.

POSTER PRESENTATION

S4-PP5

Entropy-engineered spinel-type mixed oxides for photocatalytic oxygen evolution reaction

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Entropy materials characterized by their high compositional and structural complexities introduce a transformative opportunity in photocatalysis especially for boosting oxygen evolution reaction (OER) rates in sustainable hydrogen production [1,2]. Entropy plays a pivotal role in electro/photo catalytic processes, and extensive research endeavors are dedicated to unraveling the intricate interplay among compositional-structural-entropy relationship that defines the reaction pathways [3,4]. Here we study the correlation between compositional, structural engineering and optimization of the photocatalytic oxygen evolution behaviors of medium and high entropy spinel-type mixed oxides. By elucidating the influence of metal cation composition on the photocatalytic performance of complex developed materials, we pave the way for the rational design and engineering of high-performance photocatalysts for sustainable energy transition from fossil fuel to renewable energy-based applications. Structural, morphological, optical and magnetic properties of the synthesized materials were determined via a set of complementary analytical techniques suh as: powder X-Ray Diffraction (XRD), Field-Emission Scanning Electron Microscopy (FE-SEM) and Energy-Dispersive X-ray spectroscopy (EDS) elemental mapping, Ultra High-Resolution Transmission Electron Microscopy (UHR-TEM) and X-ray Photoelectron Spectroscopy (XPS). Vibrating sample magnetometry (VSM) is further used to investigate the magnetic properties. Moreover, we assessed and compare the photocatalytic oxygen evolution performance of synthesized materials to those of the lower entropy mixed oxides ranging from binary to hexanary metallic cationic components. The present study contributes to the growing of this exciting and rapidly evolving field of research on entropy-engineered spinel-type mixed oxides and highlights their potential as versatile platforms for advanced photocatalytic applications.

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References:

[1] J. Baek, et al., Nat. Commun. 14 (2023) 5936.
[2] Q. Ding et al., Nature 574 (2019) 223.
[3] C. M. Rost et al., Nat. Commun. 6 (2015) 8485.
[4] Y. Han, et al., App. Catal. B (2023) 123096.

POSTER PRESENTATION

S4-PP6

Photocatalytic activity of composite materials based on ZnO and CuO commercial powders

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Textile industry is one of the most polluting industries of surface water, some industrial processes involved in this industry releasing significant amounts of organic compounds (for example dyes) into the wastewater, which finally lead to environmental pollution. Many studies were reported on this topic, the dyes used in the textile industry being considered to be one of the most important cause of water contamination [1]. Water pollution has harmful effects on humans and wildlife (e.g. fish) [2]. In this regard, researchers are making continuous efforts to develop efficient photocatalysts based on semiconductors under natural solar irradiation. The literature presents various n-type semiconductor such as ZnO and TiO2 used to develop photocatalysts for dye degradation [3, 4]. It is known that unmodified zinc oxide is not considered a photocatalyst with high photocatalytic activity under visible light [5] because it has a band gap at ~3.37 eV [6] and since it has a high recombination rate of charge carriers [7]. Numerous studies have shown that the heterojunction between different metal oxides improves the stability and reduces the resistance to charge transfer in the particles. For example, by coupling ZnO (n-type) with another metal oxide (p-type) a change in the band gap can be obtained and thus lead to the separation of electron-hole pairs under irradiation and therefore electron-hole recombination can be avoided [8].

In this context, the present paper is focused on the investigation of photocatalytic activity of these composites, using Rhodamine B solutions' degradation under solar light irradiation in the presence of prepared ZnO-CuO composites. The composites based on commercial powders of ZnO and CuO were prepared by mixing using a pestle and mortar for 10 minutes. The samples were structurally investigated by X-ray diffraction. The surface morphology and elemental analysis of the composites based on ZnO and CuO were explored by scanning electron microscopy. Regarding the photocatalytic activity under sunlight, investigations were made for the degradation of Rhodamine B using metal oxide composites.

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References:

[1] F.M.D. Chequer, et al., Eco-Friendly Textile Dyeing and Finishing 6 (2013) 151–176.
[2] I. A. Saleh, et al., Technol. Innovation 19 (2020) 101026.
[3] M.A. Gatou, et al., Water 15 (2023) 2773.
[4] M. Lal, et al., Res. Eng. 17 (2023) 100890.
[5] I. Zgura, et al., Materials 16 (2023) 1153.
[6] C. Florica, et al., Mater. Lett. 170 (2016) 156–159.
[7] A. Das, et al., Mater. Chem. Phys. 263 (2021) 124431.
[8] W. Ouyang, et al., Adv. Funct. Mater. 29 (2019) 1807672.

POSTER PRESENTATION

S4-PP7

Development and optimization of a microfluidic device for exosome filtration

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The purpose of the device from this work is to filter out the exosomes from blood in order to analyze them with a highly sensitive biosensor based on graphene derived materials. Exosomes in the blood carry out important genetic information related to the nucleic acids and proteins of the cells from which the exosomes were released, thus making them important possible cancer biomarkers. The working principle of the device consists as follows: the fluid is introduced in the device using two inlets (on one inlet particles are introduced, on the other just fluid) and flow focusing is used to have the particles in the near vicinity of the interior wall of the microchannel; Dean Flow is generated by the spiral microchannel to have secondary flows, the purpose here is to have a mixed two-phase flow in which the rapid phase will attract the larger particles from blood; next, at the outlet the pillar array using DLD (deterministic lateral displacement) is employed to further separate the cells from the blood to their designated exit.

In this work we perform several numerical simulations, using the commercial code Comsol Multiphisics, to assess the optimum design that filters out exosomes directly from a sample. Three types of particles are introduced from first inlet: red blood cells (d1 = 5um), platelets (d2= 1.8 um) and exosomes (d3 = 0.1 um). The optimization process considered various parameters to enhance the device`s performance. The results of the simulations offer insights into the device`s effectiveness in isolating exosomes directly from blood samples, with implications for improved cancer biomarker detection and diagnostic applications.

POSTER PRESENTATION

S4-PP8

Low metal loading supported on MAX Phases for selective hydrogenation of cinnamaldehyde

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The chemoselective hydrogenation of a functional group, when multiple functionalities are present in a molecule, is not trivial because the thermodynamic driving forces may be very similar. To address this problem, the use of heterogeneous catalysts that can chemoselectively conduct to the desired reaction has been explored. A chemoselective catalyst should recognize and interact preferentially with one functional group while avoiding the transformation of others.

Cinnamaldehyde (CAL) is a representative molecule for unsaturated aldehydes and is a compound widely found in cinnamon bars. Chemoselective reduction of CAL to the appropriate reaction products, cinnamyl alcohol (COL) or hydrocinnamaldehyde (HCAL) using suitable heterogeneous catalysts is highly desired as the homogeneous synthesis procedure is hazardous and produces waste. [1, 2]

MAX phases are ternary early transition metal carbides/nitrides with a layered hexagonal crystal structure. [3, 4] MAX phases are particularly unique because they combine the properties of metals and ceramics. In a recent study, we have demonstrated MAX phase-induced chemoselectivity in the chemoselective hydrogenation of 4-nitrostirene to 4-aminostirene. [5]

In this work, we developed MAX phase-based catalysts for the chemoselective hydrogenation of cinnamaldehyde. Indeed, the results obtained in this research indicate that MAX phases (Ti_3SiC_2, Ti_2AlC, Ti_3AlC_2) can chemoselectively hydrogenate CAL to HCOL with high selectivity (80%) but relatively moderate conversion in good agreement with our previous results. [5] In order to maintain its preferential selectivity and to enhance conversion, the MAX phase was used as a support for different Pd and Ni loadings, of 0.1 wt. % and 10 wt. %, respectively. As expected, the conversion increased up to 100%, while chemoselectivity was preserved.

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References:

[1] E. A. Redina, et al., Eur. J. Org. Chem. 26 (2019) 4159–4170.
[2] I. P. Query, et al., J. Org. Chem. 76 (2011) 6452–6456.
[3] M. W. Barsoum, T. El-Raghy, J. Am. Ceram. Soc. 79 (1996) 1953–1956.
[4] M. W. Barsoum, Wiley-VCH Verlag GmbH Co. KGaA: Weinheim, Germany, (2013).
[5] M.M. Trandafir, et al., ACS Catal. 10 (2020) 5899–5908.

POSTER PRESENTATION

S4-PP9

Transport mechanisms in IGZO memristor

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Memristors represent a novel passive electronic component with potential applications in the future, particularly in fields such as neuromorphic computing and camera surveillance. Additionally, they present a promising solution for creating an ultrahigh density memory device that can be seamlessly integrated directly onto the processor chip.

Two IGZO target composition were used for the study, first with atomic ratio In:Ga:Zn of 8:2:1 and second with In:Ga:Zn ratio of 4:1:1. Indium-Gallium-Zinc Oxide (IGZO) micro-memristors have been fabricated using photolithography and magnetron sputtering techniques. Current-voltage and current-time characteristics were performed for the obtained devices, revealing changes in resistive state of IGZO layer of various thicknesses (from 30 nm to 80 nm). It was evidenced that the changing of resistance starts from a threshold writing voltage taking values from 1.5 to 2 V. The free carrier density and mobility were extracted form Hall effect measurements, being evaluated to 8.4x10^19cm^-3 and 2.5 cm^2/Vs. After thermal treatment these values are significantly changed.

The current vs. temperature measurements showed a sqrt(T) dependence and a metallic-to-semiconductor transition which is consistent with the theory of disordered systems. Moreover, the presence of negative differential resistance (NDR) can be connected to either reversible metal-semiconductor transition or either to strongly correlated insulators, which often display multivalued I–V characteristics with regions of NDR. The above transport mechanisms are discussed and confronted to the empirical results obtained on IGZO micro-memristors.

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POSTER PRESENTATION

S4-PP10

2D Ti_3C_2Tx MXene as electrode on all oxide capacitors deposited by spray coating method

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MXenes [1] are layered 2D materials exfoliated from a bulk MAX phase - carbide/nitride (X=C/N) with an early transition metal (M) and group 13 and 14 element (A). $Ti_3C_2T_x$ MXene is particularly interesting for many reasons: water miscibility, colloidal stability, stable electronic properties [2]. The high volumetric capacitance (about 2850 F cm^{-3}) [3] and excellent electrical conductivity (20-25 kS cm-1) [4] of 2D $Ti_3C_2T_x$ MXene has made them promising materials for a wide range of applications: energy storage 5, wearable electronics [6], catalysis [7].
The goal of this study is to demonstrate the great potential of MXenes as conductive electrodes on all-oxide capacitor structures. Therefore, thin films of $Ti_3C_2T_x$ flakes were deposited on epitaxial thin film of $PbZr_{52}Ti_{48}O_3$ which was epitaxially grown on two different substrates: $SrTiO_3$, (001) oriented and $SrTiO_3$-Si, both with $SrRuO_3$ as the bottom electrode. The study aimed to optimize the spray-coating parameters to achieve uniformity and precise control over the thickness of the MXene layer, a crucial aspect in determining the overall performance of the electrodes. Layers obtained from delaminated $Ti_3C_2T_x$ (5 mg x ml^{-1}), with consecutive spraying steps on the substrate (100 C, 3 bar N_2 pressure) were found to ensure the most suitable behavior as electrodes. Time-dependent electrode stability studies across a temperature range from 25 C to 120 C were performed, which are relevant for assessing the performance and stability of the MXene-based electrodes under various operating conditions. The findings contribute to the broader understanding of MXene-based materials in the fields of electronic devices or even as solid-state supercapacitors.

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This work was supported by Romanian Ministry of Research, Innovation and Digitization through the Core Program 2023–2026 (contract PC3-PN23080303).

References:

[1] M. Naguib, et al., Adv. Mater. 23 (2011) 4248–4253.
[2] K. Li, et al., Adv. Funct. Mater. 30 (2020) 2000842.
[3] Z. Wang, et al., J. Power Sources 448 (2020) 227398.
[4] C. Yang, et al., Adv. Energy Mater. 8 (2018) 1802087.
[5] J. Nan, et al., Small 17 (2021) 1902085.
[6] N. Li, et al., Matter 4 (2021) 377–407.
[7] I.M. Chirica, et al., J. Mater. Chem. A 9 (2021)19589–19612.

POSTER PRESENTATION

S4-PP11

Bio-compatibility of stainless steel treated with advanced surface modification techniques

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In the present study, the novel surface modification approach is designed to improve the biocompatibility of stainless steel grade 316L (SS316L) for biomedical use. The process involves various advanced surface treatment techniques, including electrochemical anodisation and non-thermal plasma treatment, to create different nano-features/morphologies on the SS316L surface. Such techniques aim to enhance the performance and longevity of implants by better integration with biological tissues.

The experimental approaches, including electrochemical anodization, were performed in order to produce various nanoporous structures on SS316L substrates. This was followed by non-thermal plasma treatment to enhance surface properties, particularly by altering the chemical composition of the surface as well as wettability. The modified surfaces were thoroughly characterized using scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray photoemission spectroscopy (XPS), and water contact angle measurements (WCA) to evaluate alterations in surface morphology, chemistry and wettability. Subsequently, biological studies, including platelet adhesion and activation, were assessed, and the potential for thrombosis and restenosis on the modified surfaces was evaluated through studies of endothelial and smooth muscle cell adhesion.

The modified samples featuring nanostructured surfaces and carefully optimized physicochemical properties demonstrated markedly superior biocompatibility when compared to their unmodified SS316L counterparts. These enhanced surfaces exhibited notable reductions in platelet adhesion, enhanced endothelial cell growth, and decreased smooth muscle cell adhesion. These improvements are largely attributed to the deliberate alterations in surface morphology, chemical composition, and wettability. The nanostructuring and optimized physicochemical properties appear to play a crucial role in enhancing the biomaterial's interaction with biological tissues, suggesting promising applications in biomedical and implantable device technologies.

POSTER PRESENTATION

S4-PP12

Overcoming obstacles and finding solutions for integrating Barium Titanate–Hydroxyapatite ceramics with uncompromised piezoelectric and biological characteristics

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The promising combination of piezoelectric and osteoconductive properties in barium titanate (BT) and hydroxyapatite (HA) has sparked interest in developing advanced synthetic bone graft substitutes capable of facilitating rapid and reliable osseointegration. This study pursued two parallel strategies for blending BT and HA materials: (i) traditional sintering of BT-HA powder blends, and (ii) magnetron sputtering to apply HA coatings onto pre-sintered BT surfaces. Across a range of BT/HA ratios (from 95/5 to 80/20 wt.%), diverse crystalline qualities (including nanocrystalline or highly crystallized states achieved through pre-annealing), particle sizes (ranging from sub-micron to micron-scale), and sintering temperatures, the persistent reactivity of BT-HA blends beyond 800 °C was noted. At higher temperatures (1000 – 1300 °C), HA decomposition occurred, leading to extensive interaction with BT and the formation of secondary phases (such as $CaTiO_3$, $Ba_2Ca(PO_4)_2$, $BaCa_6(PO_4)_4O$, $BaCa(PO_3)_4$, beta-$Ca_2P_2O_7$), resulting in significant alterations to piezoelectric and cytocompatibility (as assessed in fibroblast and osteoblast cell cultures) responses. Application of HA coatings onto sintered BT ceramics effectively preserved piezoelectric properties while providing an osteogenic-friendly surface, as confirmed through tetrazolium salt-based viability assays and microscopic cell morphology evaluations. Post-deposition annealing at temperatures of 550 and 700 °C resulted in complete crystallization of HA coatings, with no observable reactivity between BT and HA. This highlights the effectiveness of HA coating in seamlessly integrating the piezoelectric and osteogenic characteristics of both constituents, without compromising their properties.

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POSTER PRESENTATION

S4-PP13

Monovalent silver complexes based on phosphine ligands designed to promote synergistic antitumor effects

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Cisplatin is widely used in cancer chemotherapy and firstly confirmed by FDA since 1978 [1]. Although the widespread success of these platinum drugs in the treatment of several solid malignancies, it is characterized by significant setbacks which minimize its usefulness. In the search of metal-based antitumor drugs alternative to platinum based chemotherapeutic agents, group 11 metal derivatives have shown encouraging results. 10 new complexes based on silver (I) were synthesized by the ligand exchange reactions by nucleophilic attack under a controlled nitrogen atmosphere. Using different types of phosphines, the silver (I) compounds were divided into two families: 5 heteroleptic complexes of the general formula $[HB(pz)_3Ag(PR_3)]$ and 5 homoleptic complexes of the formula $[Ag(PR_3)_4]BF_4$ [2]. The purity of these complexes was confirmed by elemental analysis, 1H, 13C, 31P NMR, mass spectrometry and infrared spectroscopy. The anti-cancer activity of these compounds was tested by cell culture using different human cancer cell lines. It was clear that all tested complexes were able to overcome cisplatin resistance and inhibit thioredoxin reductase activity.

References:

[1] T.C. Johnstone, et al., Chem Rev. 116 (2016) 3436–3486.
[2] K. Dammak, et al., Molecule 25 (2020) 5484.

POSTER PRESENTATION

S4-PP14

Bone graft substitutes fabricated by robocasting from bioactive and piezoelectric ceramics: Pilot studies at the National Institute of Materials Physics

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Synthetic bone substitutes (SBS) are currently regarded as possible alternate solutions, capable of bypassing a series of important adverse effects of biological bone grafts, such as (i) morbidity derived from bone harvesting, additional pain, more complex surgical procedures, limited bone material, and onsite infections, (ii) higher risk of infection and lower structural strength, and (iii) high immunogenicity risks in the case of autografts, allografts, and xenografts, respectively [1]. Additive manufacturing has emerged as a viable option for fabricating SBSs because it enables precise control over the shape, morphology, and porosity of the printed constructs. Notably, robocasting, a technology within the Direct Ink Writing family, has recently emerged as a proficient technique for producing ceramic scaffolds with desired geometry and tunable properties [2]. Robocasting technology involves an inexpensive, free-form, room-temperature process. It is based on the extrusion of ceramic suspensions with powder loading of approximately 50 - 65 vol.%, organic additives constituting less than 1 vol.%, and volatile solvents, most often water, comprising around 35 - 50 vol.%. This process yields near-shape printed objects.

This work summarizes the progresses achieved thus far at the National Institute of Materials Physics in the fabrication and multi-parametric - physical-chemical, mechanical and in vitro biological - assessment of macro-porous robocasted ceramic scaffolds. These constructs were derived from from single (Mg or Sr) and doubly (Mg and Sr) substituted bioactive biphasic calcium phosphate [3] and piezoelectric binary system $BaZr0.2Ti0.8O3–Ba0.7Ca0.3TiO3$ (BCTZ50) [4] ceramics. Through collective assessment, the results suggest definite possibilities for such robocasting-printed macro-porous scaffolds to be implemented as viable future solutions for osseous tissue reconstruction and substitution.

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References:
[1] C.E. Gillman, A.C. Jayasuriya, Mater. Sci. Eng. C 130 (2021) 112466.
[2] A. Entezari, et al., Adv. Healthc. Mater. 8 (2019) 1801353.
[3] C. Besleaga, et al., J. Funct. Biomater. 13 (2022) 123.
[4] L. Nedelcu, et al., Materials 16 (2023) 901.

POSTER PRESENTATION

S4-PP15

Temperature annealing effect on ZTO-TFT transistors performances

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Amorphous oxide semiconductors containing indium such as Indium Gallium Zinc Oxide (IGZO) have been extensively used for their several advantages, as high electron mobility and transparency. However, despite its advantages, they present a key challenge for mass production in electronic industry. As a competitive alternative material that has gained popularity in recent years, Zin Tin Oxide (ZTO) films are appealing active layers due to their elemental earth-abundance, low cost, environmental stability, good transparency and high mobility. These properties make it a promising candidate for advanced electronic applications, including high-resolution displays, solar cells and flexible electronic devices.

In this work, bottom gate conventional thin film transistor structure with an amorphous ZTO channel layer and Indium Tin Oxide (ITO) source and drain electrodes was prepared using photolithography and RF magnetron sputtering on a Si/SiO_2 substrate. Subsequently, the transistor underwent treatment at various annealing temperatures to investigate its influence on the electrical properties of ZTO thin film. The ZTO TFT I-V curves were characterized using semiconductor parameter analyzer. The electrical performance demonstrated a significant temperature dependence during annealing. The ZTO TFT annealed at 450 °C for one hour in air exhibits the best performance. It exhibits a high carrier mobility of almost 20 cm^2/V, high on/off current ratio (Ion/off) of 10^6, threshold voltage (Vth) of 2.9 V and a good subthreshold slope (SS) of 0.34 V/dec.

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POSTER PRESENTATION

S4-PP16

Investigating the influence of titanium and rhenium oxidation states on the catalytic properties of Ti–Re–O$_x$-doped materials in carbohydrate conversion to levulinic acid

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The influence of the oxidation state of titanium and rhenium within Ti–Re–Ox active species on the acid properties of rhenium-doped titania materials was a focal point of this study. Additionally, the catalytic activity of TiO$_2$, 2%Re–TiO$_2$, and 10%Re–TiO$_2$ in converting carbohydrates into levulinic acid under autoclave conditions was thoroughly evaluated. These materials were prepared using the aerogel method for the first time to the best of our knowledge and underwent comprehensive characterization using XPS, SEM-EDX, DRIFTS, DR UV-vis, Raman, N2 adsorption/desorption isotherms, TGA, and XRD techniques. Furthermore, the surface acidity was probed by NH$_3$-TPD and pyridine-FT-IR analyses. The study revealed that increasing the amount of rhenium doped into TiO$_2$ led to an increase in the total number of acid sites (Lewis + Brønsted), albeit with an overall lower strength. The presence of both Brønsted and Lewis acid sites suggested that these materials may be well suited for the conversion of carbohydrates into levulinic acid. Notably, a levulinic acid yield of 57% was achieved over 10%Re–TiO2 at a low mass ratio catalyst to glucose (1:5). Moreover, the 10%Re–TiO$_2$ catalyst demonstrated sustained catalytic activity over four cycles of glucose conversion without significant deterioration. Nano-particles including TiO$_2$, 2%Re–TiO$_2$, and 10%Re–TiO$_2$ were synthesized using a modified aerogel method, marking a novel contribution to the field. These materials were then evaluated as solid acid catalysts for the conversion of glucose or cellulose to levulinic acid at temperatures of 180°C or 210°C.The physico-chemical characterization of these catalysts, conducted extensively using various techniques, highlighted the successful insertion of Re into the titania structure and the formation of Ren+–O–Ti^{4+}(Ti^{3+}) bonds.

X-ray photoelectron spectroscopy (XPS) played a pivotal role in this investigation, providing valuable insights into the oxidation states of titanium and rhenium within the active species. The XPS spectra revealed the presence of Ti3+ and Ti4+ species, with an increasing Ti3+ intensity correlating with higher rhenium percentages. This observation suggested a potential partial charge transfer from rhenium to titanium through Re–O–Ti bonds.

Furthermore, the XPS analysis indicated the formation of Ren+–O–Ti bonds, supported by the strong metal support interaction (SMSI) property of TiO$_2$. This finding underscored the significance of rhenium doping in modifying the catalytic properties of TiO$_2$ for efficient levulinic acid production. The acid site nature on Re-doped TiO$_2$ was found to be influenced by the oxidation states of rhenium and titanium. Lewis acid sites, represented by Ti^{4+}, Ti^{3+}, and Re^{n+}, were complemented by the generation of Brønsted acid sites on the surface of 10%Re–TiO$_2$. These Brønsted acid sites, facilitated by the high oxidation states of rhenium (Re^{6+}, Re^{7+}), attracted hydroxyl ions to neutralize excess charge from Ti^{4+} ion substitution. The catalytic performance of these materials was significantly enhanced upon doping TiO$_2$ with rhenium up to 10% weight. This enhancement was attributed to the synergistic effect between Brønsted and Lewis acid sites, resulting in a remarkable increase in levulinic acid yield from 27.2% to 57%. Additionally, the presence of Ren+ species contributed to improved anatase phase stability at high temperatures, suggesting potential avenues for future research in material development and exploration in other catalytic processes.

POSTER PRESENTATION

S4-PP17

Exploring antioxidant capacities and cellular effects of spring green's polyphenolic extracts

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During spring, the human body experiences significant demands to adapt to changes in nature and the environment. A balanced diet centered around spring vegetables can aid in this rapid adaptation, as these vegetables are rich sources of energy, vitamins, fibers, and minerals that bolster the immune system. They provide an energizing, detoxifying, and antioxidant effect, aiding recovery from the harsh winter conditions and the resulting dietary deficiencies. To evaluate the antioxidant capacity of seven commonly consumed spring greens, their polyphenolic content was extracted using ultrasound-acidified methanol. Antioxidant molecules function by neutralizing free radicals through electron transfer, involving oxidation of the antioxidant molecule and subsequent reduction or neutralization. Analysis of lettuce, basil, dill, orache, parsley, ramsons, and lovage revealed variations in their effects on cell cultures despite similar overall antioxidant capacities. Lettuce displayed an antioxidant effect, whereas lovage exhibited toxicity in the same cell cultures.

The DPPH assay and spectrophotometric evaluation at 520 nm determined the antioxidant capacity of the vegetables, with EC50 values indicating the concentration necessary for a 50% decrease in DPPH radical absorbance, meaning also that this is the concentration necessary to neutralize half amount of the free radicals. Additionally, amperometry at fixed potentials of 0.3 V and 0.7 V assessed high antioxidant content and total antioxidant fraction, respectively. The lowest EC50 values correlated with the highest current oxidation peaks, confirming the antioxidant capacities measured by both methods. Further, the extracts at EC50 concentrations were evaluated in L929 cell culture, a fibroblastic cell line, revealing that, with the exception of lovage, in the case of most plants, the polyphenolic extracts promote viability and have a protective effect against oxidative stress induced by LPS and TNF. These findings emphasize that although spring vegetables may have comparable antioxidant capacities, their effects on cell cultures vary. Thus, it`s important to consume with moderation the plants with high polyphenolic content and to thoroughly assess the effects of each plant before considering them for dietary supplementation or therapeutic use. Several polyphenolic plant extracts were used for the development of polymer nanofiber scaffold with antioxidant properties. The biocompatibility of the antioxidant enriched scaffold was tested in vitro using the fibroblasts L929.

POSTER PRESENTATION

S4-PP18

Electrospun polymeric fibers doped with natural anthocyanins for monitoring pH changes

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Anthocyanins are a class of water-soluble flavonoids widely present in fruits and vegetables. Natural sources of anthocyanins include red and purple berries, grapes, apples, plums and cabbage between others. Anthocyanin molecules will change their color through a process called halochromism depending upon the pH of their environment thus it may serve as a pH indicator. The anthocyanin turns red-pink in acids (pH 1-6), reddish-purple in neutral solutions (pH 7) and green in alkaline or basic solutions (pH 8-14) [1].
pH affects most chemical and biological processes in water therefore is it is one of the most important environmental factors. pH and texture (hardness) are major factors that affect the quality of food. The pH affects the pigment, taste, texture, and shelf life of food, and rapid changes can have undesirable effects on food.

The change of pH will lead to the ionization of amino acids atoms and molecules, change the shape and structure of proteins, thus damaging the function of proteins.

The pH of meat is an important factor that determines the freshness, taste and overall quality of meat. In a meat sample, intrinsic parameters such as pH, water-binding capacity, presence of salts and temperature determines its palatability, freshness and potential to develop microbial growth. pH refers to the level of acidity or alkalinity in meat, and it plays a crucial role in determining the quality of the meat [2]. Monitoring pH throughout storage enables producers to determine the appropriate storage time and temperature conditions to maintain meat quality and safety.

This work proposes a new colorimetric sensor in order to monitor the change in meat pH using natural anthocyanins. As a matrix for these pH indicator electrospun PMMA fibers were use [3]. The obtained doped fibers were characterized by UV-Vis spectroscopy, RAMAN spectroscopy and Scanning Electron Microscopy.

In order to prove the applicability of the proposed material colorimetric tests between pH 3 to 9 were performed.

References:

[1] S. Chen, et al., International Journal of Biological Macromolecules 149 (2020) 271–280.
[2] H. Jankowiak, et al., European Food Research and Technology 247 (2021) 2813–2820.
[3] A. Aldea, et al., Microchemical Journal 165 (2021) 106108.

POSTER PRESENTATION

S4-PP19

Study on the influence of reaction compounds on the size distribution of gold nanoparticles (AuNp)

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The aim of this study was to investigate the synthesis conditions on the size distribution of gold nanoparticles and to correlate their size with their functionalization with different ligands, playing an essential role for the development of virus-like particles. Gold nanoparticles were synthesized using gold chloride trihydrate (which, upon reduction of gold ions forms the core of the nanoparticle) and trisodium citrate dihydrate (which provides the citrate groups that form stabilizing coat for the individual nanoparticles). Addition of tannic acid, which serves as a reductant for gold ions [1], was shown to play an important role in determining the size of gold nanoparticles. In order to obtain different sizes of synthesized gold nanoparticles three different volumes of tannic acid were added: 47, 50 and 52 µL. It is important to study whether nanoparticle size can be influenced by other parameters such as concentration and number of washes. Thus, the obtained gold nanoparticle solutions were diluted 4 and 8 times and washed 3 times before characterization.

UV-Vis absorption spectra of gold nanoparticle solutions (concentrated, diluted and washed) were analyzed. Scanning electron microscopy (SEM) technique was used to characterize the morphology of gold nanoparticles. The size of the gold nanoparticles was obtained analyzing the images with the ImageJ software. Nanoparticles with sizes between to 11-13 nm were selected for functionalization with different ligands such as PEG or mercaptobutyric acid. The nanoparticles-ligand assemblies were characterized by UV-Vis spectrophotometry, scanning and transmission electron microscopy and will be further used in assemblies with capsid proteins to mimic the virus shell [2].

References:

[1] B. Dragnea, et al., J. Am. Chem. Soc. 125 (2003) 6374–6375.
[2] C. Chen, et al., Nano Lett., 6 (2006) 611– 615.

POSTER PRESENTATION

S4-PP20

Polyimines designed for trifluoroacetic acid detection: promising materials for waveguide interferometer sensors

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Trifluoroacetic acid (TFA, CF_3COOH) as a volatile perfluorinated carboxylic acid belongs to the class of per- and polyfluoroalkyl substances (PFAS). Long-chain PFASs were identified to cause adverse effects on human and animal health, to be persistent in the environment, and to affect the food chains [1]. The unintentional exposure of population to PFASs was linked with various cancers, reduced immune and liver responses, high cholesterol level, or birth defects [2]. Being refereed as "forever chemicals", largely used in commercial and industrial products, PFASs can withstand extreme temperatures and are resistant to water and grease. The list of PFASs enlarged over the time, and many investigations have focused on shorter-chain PFASs, which are proposed to replace the long-chain counterparts. However, these also proved to have widespread environmental occurrence and similar concerns [3].

TFA is the longest-chain PFASs that degrade and accumulate in environmental aqueous phases, being observed in significant and increasing quantities in surface water, rain, fog, sewage treatment plants, snow, atmosphere, and sediments. Deposits of TFA (mainly as anions) with precipitation (rain and snow) can lead to its presence and accumulation in the aquatic and cryosphere environments, leading to the depletion of the ozone layer and other unknown long-term environmental consequences [4]. Thus, the TFA detection methods are imperative to be developed to reduce the environmental impact and other associated effects.

Imine-based derivatives have demonstrated great capability for TFA detection by colorimetric or fluorescence methods [5], therefore their potential can be extended to photonic sensors operating on different principles of detection. Here, we report on the design, synthesis and investigation of triphenylamine-based polyimines towards using as sensing materials for TFA detection. The influence of the structural motif on the sensing ability is discussed, with emphasis on the polymers' potential as sensing coatings in waveguide interferometer sensors.

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References:

[1] R. A. Dickman, D.S. Aga, J. Hazard. Mater. 436 (2020) 129120.
[2] E.C. Bonefeld-Jorgensen, et al., Cancer Causes Control 25 (2014) 1439.
[3] M.d.l.A. Garavagno, et al., Sustainability 16 (2024) 2382.
[4] F. Freeling, M. K. Björnsdotter, Curr. Opin. Green Sustain. Chem. 41 (2023)100807.
[5] X. Niu, et al., J. Mol. Str. 1259 (2022) 132754.

POSTER PRESENTATION

S4-PP21

Development of an electrochemical biosensor for the evaluation of enzymatic activity of methionine sulfoxide reductase A

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The study of structural modification in peptides and protein induced by oxidation of amino acid residues have been involved in different pathological conditions such as cancer or neurodegenerative diseases. Methionine residues are very prone to oxidation and the oxidation mechanism of its side chain in proteins or peptides is dictated by oxidizing species, protein structure or solvent properties. The oxidation of methionine (Met), acetyl-methionine (Ac-Met) and a series of synthetic peptides, Ac-Gly-Met-Gly, Ac-(Gly)$_2$-Met-(Gly)$_2$ and Ac-(Gly)$_3$-Met-(Gly)$_3$ was investigated by differential pulse voltammetry, in a wide pH range, at glassy carbon electrode and an oxidation mechanism was proposed. The obtained results revealed that the first oxidation step consists in one-electron oxidation of thioether component leading to the formation of a cation radical. Following this, according to the experimental conditions and the side chain position of methionine, the formed radical can be stabilized by the nucleophilic attack of water molecules or by catalytic support of the neighboring carbonyl and amide groups in an intermediate structure, finally converted in methionine sulfoxide which can be further oxidized, at more positive potential, into methionine sulfone. For methionine, at acid media, and for Ac-(Gly)3-Met-(Gly)3, at high alkaline media, the amino and amide groups are active involved in the oxidation process and the electrode reaction take place with proton transfer.

The main objective of this study consistS in the development of an electrochemical biosensor to detemine the evaluation of the enzymatic activity of methionine sulfoxide reductase A (MsrA), enzyme with an important role in Alzheimer's disease and which can be exploited for the development of tools for early diagnosis of this neurodegenerative disease. Forwards, in order to evaluate the activity of methionine sulfoxide reductase, a biosensor based on Ac-(Gly)$_3$-Met(O)-(Gly)$_3$ and screen-printed electrodes modified with zinc oxide nanowires was developed. The ZnO nanowires was prepared by electrochemical deposition performed in a double-wall electrochemical cell equipped with a recirculating thermostatic bath operating at 90 °C. The obtained nanowires were characterized from the morphological point of view. The utilization ZnO nanowires revealed an important increase in selectivity of the designed biosensor. The regeneration capacity of this biosensors was evaluated through voltammetric techniques.

POSTER PRESENTATION

S4-PP22

PLD-based pyramidal-shaped ceria biointerfaces

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Cerium oxide`s ability to switch oxidation states according to changes in environmental conditions has made it a vital component of a wide range of applications. For the first time, this work presents a pyramid-shaped nanostructured ceria film obtained by Pulsed Laser Deposition (PLD), aimed at triggering early responses in mammalian cells, as well as the detection of the enzyme cofactor nicotinamide adenine reduced dinucleotide (NADH). By varying the number of pulses, scanning electron microscopy and atomic force microscopy images of the nanostructured surfaces demonstrated shapes ranging from quasi-pyramidal to sharp edges with dimensions up to 350 nm. A correlation was found between the topographical characteristics and the transition from hydrophobic to moderately hydrophilic behavior for samples with more prominent features. By observing differences in early adhesion and distribution of phenotype SaOs-2 cells, pyramidal-shaped ceria was demonstrated to influence the in vitro biological performance of SaOs-2 cells. For the purpose of comparing cytoskeleton responses to the different ceria nanostructure types, mesenchymal stem cells (MSCs) were used since adhesion and spreading are cell line-specific. It is foreseen that the behavior of mesenchymal progenitor cells will be studied in view of establishing the osteogenic response to these biomaterials, and the most appropriate processing method will be chosen to use them in future bone regeneration applications.

Using a PLD-deposited CeO_2 oxide layer and electrochemical mediators, modified C electrodes were employed for the fabrication of stable (acidic and basic) sensors for NADH detection and biosensors based on NAD+-dependent dehydrogenases. CeO_2 coatings can be created by PLD using the technique as a way to deposit compact and nanostructured surfaces, control the thickness of the coatings over the entire surface of the substrate, and ensure high stability within liquid environments. In addition, droplet modification with a suitable mediator, such as syringaldazine, strongly adsorbed on the ceria layer, can be combined to obtain a stable sensor that is more selective and less susceptible to interference in real samples by lowering the potential value necessary to oxidize the compounds. The development of PLD-modified carbon electrodes with nano- and micropyramidal structured CeO_2 oxide thin layers for the detection of NADH and substrates of NAD+-dependent dehydrogenases provides an essential tool in food quality control and bioanalysis.

POSTER PRESENTATION

S4-PP23

Gas sensing studies using polyaniline-coated chemiresistive sensors subjected to electron beam irradiation

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In the present paper, we have investigated the effect of different doses of electron beam irradiation on the gas-sensing properties of polyaniline (PANI) film-based chemiresistor-type sensors for methane (CH4) sensing applications. The PANI sensing film was synthesized directly onto the sensor gold-interdigitated electrodes by chemical oxidative polymerization [1]. The obtained PANI-coated sensors were firstly used to detect CH_4 concentrations ranging from 1 to 100 ppm and afterward were subjected to electron beam irradiation at the irradiation doses of 50, 100, 150, 200 and 250 kGy. Irradiation was performed in atmospheric conditions and at room temperature of 25°C using the electron linear accelerator of 5.5 MeV, ALID 7 from the National Institute for Laser, Plasma and Radiation Physics, Magurele, Romania [2]. The nominal values of the electron beam parameters were: energy of 5.5 MeV, peak current of 130 mA, output power of 134 W, pulse duration of 3.75 μs and pulse repetition frequency of 50 Hz [3]. The irradiated PANI-coated sensors were subsequently employed to detect the same CH_4 concentrations. Hence, sensor performance parameters (i.e. sensitivity, limit of detection, response time, recovery time, etc.) for all prepared samples were determined.

Moreover, we have analyzed the structural and morphological properties of these PANI films, by scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS) measurements, before and after electron beam irradiation. In conclusion, depending on the irradiation dose, the effect of electron beam irradiation causes both chain scission and cross-linking processes in PANI, further influencing the sensor performance parameters.

POSTER PRESENTATION

S4-PP24

In vitro enhancement of antitumor drug efficacy by magnetic field-assisted rotation of gold-coated magnetic nanoparticles

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Cancer is the second leading cause of death worldwide, accounting for about 9.6 million deaths in 2018 [1] and 18.09 million diagnosed cases in 2020 [2]. Remote magneto-mechanical actuation (MMA) of magnetic nanoparticles (MNP) is emerging as a promising therapy method in oncology [3]. However, translation to the clinic faces the challenge of whole-body action and the reluctance about indiscriminate mechanical action of the nanoparticles on tumor and healthy cells. Here, we show that gold-coated iron oxide nanoparticles (Au@MNP), subjected to remotely-applied low-frequency rotating magnetic fields, represent one of the most efficient, simple, and convenient ways to increase the antitumor activity of an antitumor conventional drug (mitoxantrone, MTO) against tumor cells. While reports are showing biogenic gold nanoparticles as effective in killing cancer cells, our results show that synthetic Au@MNP do not affect tumor cells directly by themselves, but only if rotated by magnetic fields and synergistically with the antitumor drug, stimulating the activity of the latter. This result has a significant impact on the clinical translation of MMA, considering that the current oncology practice would not need critical adaptation in terms of procedures, doses, and schedule of drug administration. Moreover, taking into account that during the process of metastasis, circulating cancer cells resist mechanical destruction induced by hemodynamic forces and are therefore potentially more robust to the mechanical forces exerted by rotating/vibrating magnetic particles, this approach could also prove beneficial during metastatic spread.

In perspective, the use of nanoparticles loaded with antitumor drugs, capable of progressive drug release, in full dependence on the nanoparticles' rotation speed, could further provide improved alternatives for oncological therapeutic applications. Practically, a significant advance in oncology therapy can be expected by implementing such an approach, which would allow a significant decrease in the drug concentration, while maintaining the antitumor effects at therapeutic levels or, alternatively, maintaining the drug concentration at current doses, but with systemic increase of therapeutic efficiency. Moreover, the current oncological protocols shouldn't be fundamentally changed, as mentioned.

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References:

[1] https://www.who.int/health-topics/cancer#tab=tab_1.
[2] https://www.wcrf.org/cancer-trends/global-cancer-data-by-country.
[3] C. Naud, et al., Nanoscale Advances 2 (2020) 3632–3655.

POSTER PRESENTATION

S4-PP25

Study of ternary organic photovoltaic cells based on P3HT:PAni:Phen blend using the WO_3 mesoporous thin film as holes transport layer

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The rapid development of organic photovoltaic structures (OPVs) based on non-fullerene acceptors has attracted increasing attention during the past few years. This increased interest towards OPVs enables new possibilities for ternary organic solar system (TOSC). This work summarizes very recent developments of TOSCs, with a focus on blends involving non-fullerene acceptors. In ternary organic photovoltaics, the third component aligns its absorption spectrum with the binary components. It`s suggested to have a lower percentage in the blend and exhibit an infrared absorption band for improved performance. Knowing the advantages offered by the ternary compounds used as main absorber [2, 4] we prepared and characterized ternary photovoltaic cells in which the absorber layer was P3HT: PAni:Phen (1:1:0.8) blend (One Donor and Two NFAs). In this study, ternary photovoltaic based on P3HT:PAni:Phen (1:1:0.8) blend structures were fabricated by spin coating and characterized optically and opto-electronically. Also, for comparation, two transparent electrodes were used on which mesoporous WO_3 layer was deposited under ambient pressure and room temperature conditions using the PLD technique. The thickness of the layers was tuned by varying the number of laser pulses (from 36000 laser pulses to 600). Before embedding into the hole transport layer (HTL), the mesoporous WO_3 was morphological and optical characterized. The WO_3 layers consists of a highly integrated mesostructure, characterized by a uniform distribution of pores across the surface. The X-ray diffraction confirms that the WO_3 layers have a monoclinic structure with an average crystallite size of approximately 8±2 nm and a strain of 2.6±0.3 %. The results obtained demonstrated that these TOSCs are more promised structures for highly efficient solar cells. This outstanding result is attributed to the so-called “two-in-one” strategy, in which two NFAs with similar chemical structures work as an acceptor alloy, increasing the PCE of the ternary OPC as compared to the binary counterpart.

POSTER PRESENTATION

S4-PP26

Silver-coated magnetite for tumor cells treatment

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Nanotechnology has imposed itself as a potent tool in a large variety of life science and medical applications. One particular field of development for nanomedical systems is cancer therapy [1]. The so-called multimodal therapeutic approach has been recognized as a modality to increase efficiency, avoid side effects as well as the cancer relapse associated with cell heterogeneity within a tumor and metastatic dissemination [2]. Multimodal cancer therapy has benefited from noble metals such as gold nanoparticles which have shown a fine potential in backing the chemotherapy and radiotherapy treatments.

The remote magnetic actuation, constantly changes the position of the MNPs, depending on the field gradients and frequency, to generate torques onto the cells. Such torques can modify the level of calcium entry within cells, stimulate drug release from nanoparticles, induce protein degradation, and destroy cancer cells.

Our study examined the most effective combinations of chemotherapy, hyperthermia, and magneto-mechanical actuation of silver-coated magnetite nanoparticles (MNP@Ag), which were able to destroy tumor cells in vitro while maintaining the viability of normal cells [3]. We have observed that only one of the nine treatment configurations we have used satisfied both the safety requirement for normal cells (fibroblasts) and the highly cytotoxic requirement for tumor cells (HeLa), namely the combination of all three triggers. As a result of this combination, HeLa viability decreased to about 32%, while fibroblast viability decreased only to about 80%. It was observed that the cytotoxic effect was not a sum of the separate effects of each trigger involved. Instead, the triggers were conjugated nonlinearly in a dynamic regime imposed by the magneto-mechanical actuation. We conclude that chemotherapeutic drugs can be substantially reduced while maintaining their therapeutic performance by using such a treatment approach.

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References:

[1] A. Farzin, et al., Adv. Healthc. Mater. 9 (2020) e1901058.
[2] V. Manescu Paltanea, et al., Materials 14 (2021) 5948.
[3] D.D. Herea, et al., Coatings 13 (2023) 406.

POSTER PRESENTATION

S4-PP27

Tuning the wettability of poly(vinyl formal) polymer films via matrix assisted pulsed laser evaporation (MAPLE)

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The fabrication of nanostructured surfaces with tunable wettability is of high interest both in research and industrial applications, i.e., from self-cleaning and antibacterial, to antireflective and solar cells due to the excellent water-repellent properties even under severe environmental conditions.

In this work, we report on obtaining poly(vinyl formal) coatings through the matrix assisted pulsed laser evaporation (MAPLE) using a wide range of experimental deposition conditions with the aim of fabricating coatings with adjustable wettability. Within this context, we present the results of the laser fluence effect, the use of different initial deposition solutions using different solvents (i.e., chloroform: methyl alcohol, chloroform: dimethyl sulfoxide and chloroform: acetone, respectively), different concentrations of PVF in the target (i.e., from 0.25 to 10% by weight), of the morphology, topography of PVF coatings, as well as wettability properties. The as obtained polymer coatings are then tested in cell cultures (ex. BEND.3 mouse brain endothelial cell line) to evaluate their adhesive properties. This is in particular a crucial requirement for implantable porous biomaterials serving as scaffolds for tissue regeneration.

POSTER PRESENTATION

S4-PP28

Enhancing starch functionality through non-thermal plasma for innovative natural-inspired materials

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Natural polymers like cellulose, starch, and chitosan hold significant promise for application in bio-based advanced materials owing to their sustainable nature and distinctive properties. Starch, in particular, is a complex biopolymer known for its versatility, useful not just in traditional sectors like food, papermaking, and textiles, but also in emerging fields such as biomaterials, nanotechnology, and tissue engineering. However, its inherent form presents functional limitations, including low solubility in water, retrogradation, syneresis, and poor thermal and rheological properties. Radiofrequency (RF) plasma emerges as a versatile tool for tailoring the physicochemical properties of various biomaterials, including starch, altering its solubility, viscosity, molecular weight, and polymerization degree. This offers potential solutions to starch limitations. Tailored modifications are achievable by controlling both starch and plasma parameters, enhancing functionality for specific bio-based material applications. Hence, this study focuses on the influence of several input variables in starch functionalization using the RF plasma technique. Thus, starch samples were exposed to low-pressure RF plasma, with variations in sample quantity, initial moisture content, vacuum level, RF power, and treatment duration. Subsequent evaluations included characteristics such as water content, pH, solubility, apparent viscosity, molecular weight distribution, etc., for treated samples. Results revealed a direct impact of both material and processing variations on modification and functionalization efficiency via plasma processing. The selection of input variables can determine the appearance of competitive reactions (degradation, crosslinking, or molecular rearrangement) to varying degrees, thus defining the unique properties of the modified starch. This makes it more attractive as a biomaterial for a wide range of applications, including intelligent biodegradable packaging, 3D printing products, drug delivery systems, tissue engineering scaffolds, implant coatings, medical biosensors, etc. These findings significantly contribute to expanding starch versatility by demonstrating the efficacy of RF plasma modification in developing innovative, naturally inspired materials with tailored properties.

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POSTER PRESENTATION

S4-PP29

Fabrication and characterization of improved POLY(E-CAPROLACTONE) (PCL) films for applications in biliary stents

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Biliary stents are tubes made of polymer or metal to relieve obstruction in the biliary tree, to treat biliary leaks or strictures and are also being used for palliative treatment of advanced malignancies of the biliary tract. Often, excessive growth of tumor within biliary wall and formation of biofilm on inner surface of stent can cause restenosis or even obstruction after stent implantation. Therefore, it is important and valuable to develop a new biliary stent for anti-cholangiocarcinoma and anti-biofilm formation. In this case we study polycaprolactone free standing films, fabricated with spin coating deposition methods, for the development of a new biliary stent, with good biocompatibility, completely bioabsorbable and with anti-biofilm formation.

In this work we present the results of a study investigating the effects of the experimental parameters on the morphological characteristics of Polycaprolactone (PCL) thin films produced through spin coating and matrix-assisted pulsed laser evaporation (MAPLE). Polycaprolactone is a promising, absorbable material that has been used in the manufacturing of bone implants and cardiovascular stents. The good biocompatibility, non-toxicity, and biodegradability make it an ideal biomaterial.

The polymer coatings obtained in this manner are characterized for their structural, morphological, and compositional attributes using techniques such as XRD, AFM, SEM, Raman, and FTIR. Additionally, the phenomenon of PCL layer detachment from the deposition substrate will be discussed. Lastly, laser-induced periodic surface structures were obtained in the polycaprolactone free-standing membrane layers by irradiation with linearly polarized radiation.

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POSTER PRESENTATION

S4-PP30

Anionic dye pollutant adsorption from wastewaters by layered double hydroxide calcined materia

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The dyes represent a source of water pollution. The industries that generate dye contaminated waters are textile dyeing, papermaking, printing, production of personal care products, and food processing [1]. The layered double hydroxides materials as functional adsorbents in the field of wastewaters treatment contaminated with different types of dyes (anionic/ cationic) has drawn interest [2,3]. Congo Red was selected as anionic dye contaminant model for the present research.

In our previously published study [4], it was demonstrated that layered double hydroxide calcined material synthesized by co-precipitation method followed by calcination method can be involved as adsorbent for Congo Red dye removal using an adsorbent dosage of 1 g/L. The researchers highlighted in their studies that the adsorbent dosage has a significant impact on the adsorption performance of the material used [5]. Therefore, the main purpose of this research was to investigate the adsorption of Congo Red dye using a lower adsorbent dosage (0.5 g/L). The experiments were performed at ~25 °C using an initial dye concentration of 30 mg/L. The contact time ranged from 5 min to 180 min. The residual concentrations were determined by a UV-Vis spectrophotometer at 497 nm. According to the results, the adsorption capacity gradually increased with the increases of contact time. Afterwards, the kinetic modelling of the adsorption data was performed using Pseudo first order kinetic model (linear and non-linear forms), Pseudo second order kinetic model (linear and non-linear forms), Intraparticle diffusion kinetic model (linear form), and Elovich kinetic model (linear and non-linear forms). The data fitted well with Pseudo second order kinetic model, indicating that the adsorption process might be controlled by chemisorption.

The findings of this study demonstrated that the layered double hydroxide calcined material showed a higher adsorption capacity at an adsorbent dosage of 0.5 g/L (43.89 mg/g) compared with an adsorbent dosage of 1 g/L (17.92 mg/g).

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References:

[1] Y. Wen, et al., Colloids and Surfaces A: Physicochemical and Engineering Aspects 688 (2024)133661.
[2] H. Starukh and S. Levytska, Applied Clay Science 180 (2019) 105183.
[3] M. Li, et al., Journal of Alloys and Compounds 976 (2024)173107.
[4] D. Gherca, et al., Applied Clay Science 233 (2023) 106841.
[5] H. K. Ibrahim, et al., International Journal of Biological Macromolecules 262 (2024) 129730.

POSTER PRESENTATION

S4-PP31

Enhancing romanian naval resilience to climate change: advanced functional materials for Green Defense strategies

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Climate change poses multifaceted challenges to the Romanian Navy, impacting operations, infrastructure, and coastal security. This paper explores the integration of advanced functional materials as a key component of the `Green Defense` approach to mitigate these challenges. We analyse the vulnerabilities of naval operations to climate stressors like sea-level rise and extreme weather. The potential of advanced functional materials – with their enhanced properties – is examined as a solution enabling adaptive technologies. These include self-healing ship coatings, high-strength composites, robust infrastructure materials, hydrophobic/antifouling materials and sensor systems optimized for early warning. Case studies highlight the potential of these materials to strengthen Romanian naval capabilities and national security in a changing climate.

POSTER PRESENTATION

S4-PP32

Spectacular dispersibility of oxide nanoparticles synthesized by laser pyrolysis with isopropanol vapors as sensitizer

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Nanofluids and nanostructures based on magnetically structures crystalline nano-domains have gained considerable attention in various applications including high density magnetic information storage devices, drug delivery, catalysts in the pharmaceutical industry, contrast elements in diagnosis, hyperthermia treatment, and many more. The low dimensionality of nanomaterials leads to an unusually high ratio between the number of atoms on the surface layers compared to those in deep, volume layers, and this leads to significant physical-chemical changes.

This paper will focus on specific experimental conditions for obtaining iron and stannous oxide nanoparticles, and the effect of the experimental parameters on the final properties of the material, including its dispersion in different fluids. Both types of NPs were synthesized with the laser pyrolysis technique. This technique is based on the interaction between a focused laser beam (CO_2 laser in quasi continuum regime) and at least one gaseous species in the precursor mixture. Iron pentacarbonyl ($Fe(CO)_5$) and Tetramethyltin ($(CH_3)_4Sn$) were used as precursors for iron oxide and stannous oxide nanoparticles, respectively. While the most common sensitizer used is ethane (C_2H_4), a weaker sensitizer (such as isopropanol) can come with the advantage that after the laser-molecule interaction the energy transfer is lower. Therefore, the C content of iron oxide samples obtained by laser pyrolysis using isopropanol as a sensitizer is lower than when ethane is used. In the case of tin oxide NPs, synthesis with isopropanol as sensitizer has a positive influence in tin dioxide formation as opposed to tin monoxide.

The elemental and structural characterizations (EDX, TEM, XRD) confirmed the nature of the particles, and DLS analysis indicated excellent stability of the samples in distilled water. Further, a reference sample was tested regarding its stability in organic fluids. The results displayed extremely reduced NP agglomerations with exceptional stability, even after 20 h. Moreover, this protocol did not hinder the magnetic behavior of the NPs.

POSTER PRESENTATION

S4-PP33

Sr-doped Hydroxyapatite/ Chitosan composite layers deposited on titanium substrates for bone tissue engineering applications

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In this work we report the deposition of hydroxyapatite and Sr-doped hydroxyapatite on mirror-like and unpolished Ti substrates by radio-frequency magnetron sputtering at different substrate temperatures, followed by the deposition of chitosan by matrix-assisted pulsed laser evaporation. The physicochemical properties of the layers were evaluated by Scanning Electron Microscopy, Energy Dispersive X-Ray Spectroscopy, Fourier Transform Infrared Spectroscopy, and X-ray Photoelectron Spectroscopy (XPS). The layers biocompatibility and cytocompatibility were evaluated by MTT, LDH, and "Live/dead" cell assays on L929 cells and the antibacterial activity was tested against Staphylococcus aureus.

The investigations revealed that the composite layers containing both Sr and chitosan are the most suitable for bone tissue engineering applications due to increased cell viability and antimicrobial properties. These findings were associatedwith the influence of the substrate temperature and surface roughness on the morphology of the coatings, as the grain-like structures, specific for the layers deposited without heating the substrates, were replaced by more compact structures at the highest deposition temperature (400 °C), for both mirror-like and unpolished Ti substrates. The presence of the Ca 2p peaks corresponding to hydroxyapatite in the high-resolution XPS spectra of the chitosan containing layers highlighted that composite coatings were obtained.

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POSTER PRESENTATION

S4-PP34

Spiking neuron based on dual-free layer magnetic tunnel junction

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The magnetic tunnel junction (MTJ) are key elements in the development of spintronic devices and offers a large panel of advantages in terms of size, energy consumption and operation speed. Their non-volatility serves to store information in magnetic random access memories MRAM and the field-dependence of their resistance allows conceiving magnetic field sensors. Beside to these well-known applications, new functionalities can be envisaged by adapting the composition of the magnetic stacks and the stimuli. One promising structure is an MTJ with two free layers capable of continuously switching their magnetization if a bias voltage is applied, thus generating trains of resistance spikes, signals similar to firing event in biologically inspired neurons. The interplay between the inter-layer coupling mechanisms and their individual parameters are responsible of various operating regimes. Modelling and experiments have been performed to identify the suitable condition for spiking. We demonstrated that spike frequency is tunable in the MHz range by varying the voltage amplitude and depends on the MTJ lateral size. The control of the spike generation as well as the downscaling of the MTJ are essential in developing artificial neurons CMOS compatible. Additionally, the device operating point at zero magnetic field is relevant for large-scale integration point of view and hardware implementation of spiking neural networks (SNN) for energy efficient computation of spatio-temporal data.

POSTER PRESENTATION

S4-PP35

Synthesis and characterization of functional properties in flexible ferroelectric composites with PVDF-TrFE matrix

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Flexible ferroelectric composites have been developed using a ceramic powder of (1-x)$SrFe_{12}O_{19}$-(x)0.92($Bi_{0.5}Na_{0.5}TiO_3$) – 0.08($BaTiO_3$) (BNT-BT) composition integrated within a matrix of poly(vinylidene fluoride-trifluoroethylene) (PVDF-TrFE). The preparation process begins by dissolving the PVDF-TrFE matrix in a 10% proportion in the suitable solvent dimethylformamide. Ceramic particles are then integrated into the solution, ensuring uniform distribution and optimal interaction of the ceramic particles within the matrix, facilitating a uniform spin coating process. The spin coating technique was employed to deposit a thin layer of this solution on Indium Tin Oxide (ITO) coated glass substrates. The resulting films are then subjected to thermal treatment at 140 °C for 2 minutes for drying.

The developed composites were structurally, microstructurally, and electrically characterized to evaluate phases, surface morphology, and functional properties. Broadband impedance spectroscopy analyses indicate an improvement in interfacial polarization and an increase in the number of internal micro-capacitors as a relaxation source. This work contributes to understanding ceramic-polymer interactions and their impact on overall performance. The results reveal the potential of PVDF-TrFE-based composites in advanced applications such as flexible sensors and actuators.

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POSTER PRESENTATION

S4-PP36

Enhancing perovskite solar cells efficiency by incorporating graphene oxide in the electron transport layer using electrochemical methods

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Nowadays, renewable energy resources are demanded to be more efficient, sustainable and low cost. Different energy storage devices (ESDs) have been developed based on the conversion of sunlight into an electrical and chemical energy such as solar cells (SCs). Typically, SCs are composed of electron transport layer (ETL) deposited on a transparent conducting oxide (TCO) layer, absorber, hole transport layer (HTL), and current collector. Perovskite has shed some photovoltaic promise as absorber layer, being considered one of the biggest scientific breakthroughs [1]. This is due to the high photovoltaic performances of solid-state SCs based on halide perovskites, which reached 9.7% in 2012, up to 17.9% in 2014, and exceeded 25% since 2020 [1]. The most efficient perovskite solar cells (PSCs) is built with a compact layer (CL) and mesoporous layer (ML) infiltrated with perovskite microcrystals, a perovskite capping layer, a hole transporting layer (HTL), and a metal electrode (full cell). CL and ML are playing a determinant role in efficiency of PSCs since the former reduce the contact resistance and the interfacial charge recombination, while the latter serves as ETL. TiO_2 and SnO_2 have been found as some of the best candidates for CL and ML [2]. Currently, PSCs fall short of meeting industrial standards due to their moderate efficiency and challenges in achieving reproducible and stable performance. To advance their development, existing synthesis methods must improve, and new routes should be explored [3].

Various strategies have been adopted in order to improve solar cells efficiency, including the engineering of the different layers and interfaces [4]. In this context, in recent years, the introduction of graphene and derivatives into PSC architecture has been proven to improve the performance and stability of SCs [5]. Graphene has exceptional properties including high electron mobility, good chemical stability, suitable energy level, and high transparency which can help to improve the solar cell efficiency [5]. In this work, we aim to engineer the ETL layer of PSCs with reduced graphene oxide (rGO). RGO are obtained by electrodeposition (ED). ED is one of the simplest, cheapest and greenest method to produce rGO [6]. Compact and mesoporous TiO_2 ETL layers are fabricated either by spray deposition method or by electrochemistry. Their synergy with rGO will be investigated through various morphological (e.g., SEM) and physico-chemical characterization techniques (e.g., Raman spectroscopy, XRD, and optical measurements). The efficiency of SCs fabricated with the modified ETLs is evaluated.

References:

[1] M. Al Katrib, et al., ACS Appl. Energy Mater. 5, (2022) 4461.
[2] H. Mohammadian-Sarcheshmeh, et al., Heliyon 4 (2018) e00912.
[3] S.L. Hamukwaya, et al., Coatings 12 (2022) 252.
[4] S. Bera, et al., Mater. Adv. 3 (2022) 5234.
[5] K. Gong, et al., Mater. Des. 211 (2021) 110170.
[6] T. Tite, et al., J. Nanobiotechnology 17 (2019) 101.