Institute of Solid State Physics
University of Latvia

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Riga 2024

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Introduction

The Institute of Solid State Physics (ISSP UL) of the University of Latvia is the main research center in the field of materials science in Latvia. It was founded in 1978 by an amalgamation of the two largest physics research laboratories in the University of Latvia: Laboratory of Semiconductor Research and Laboratory of Ferro- and Piezoelectric Research. Since 2013, the ISSP UL has the status of a legally and fiscally independent organization of the University.

To encourage more students to select physics and chemistry, in the mid-90s ISSP UL stepped-up its teaching activities. Several researchers were elected as professors at the University of Latvia. Post-graduate and graduate curricula were prepared. Presently they are offered in solid-state physics, materials physics, chemical physics, physics of condensed matter, semiconductor physics, and experimental methods and instruments.

In December 2000, the ISSP UL was awarded the **Centre of Excellence of the European Commission** (Centre of Excellence for Advanced Material Research and Technologies – **CAMART**). Together with the associated financial support of 0.7 M EUR for a 3-year duration, this award boosted our research activities and allowed us to extend the network of our research partners and scientists, who came to work at ISSP UL from the leading European research centres. In 2001 the Association EURATOM-University of Latvia was established, and the ISSP UL became the coordinator of the Latvian Research Unit. In 2014 EUROfusion consortium agreement was signed, regulating European cooperation in thermonuclear synthesis research. The 34 countries are working together to tackle the complex challenges facing a practical fusion power plant that produces electricity.

In 2015, ISSP UL was awarded the Horizon 2020 Teaming project: "**The Excellence Centre of Advanced Material Research and Technology Transfer – CAMART^2**". 169 proposals were submitted; 31 were selected to develop their Business Plans. The project scored 14.5 out of 15 points; it was the only project approved for financing from Latvia and other Baltic countries. CAMART^2 was submitted in cooperation with Swedish partners from the Royal Institute of Technology (KTH) and the Research Institute of Sweden (RISE). The Business Plan was highly estimated in the second phase of the Teaming project, dedicated to the development of the Centre of Excellence during 2017-2024 (Figure 1).

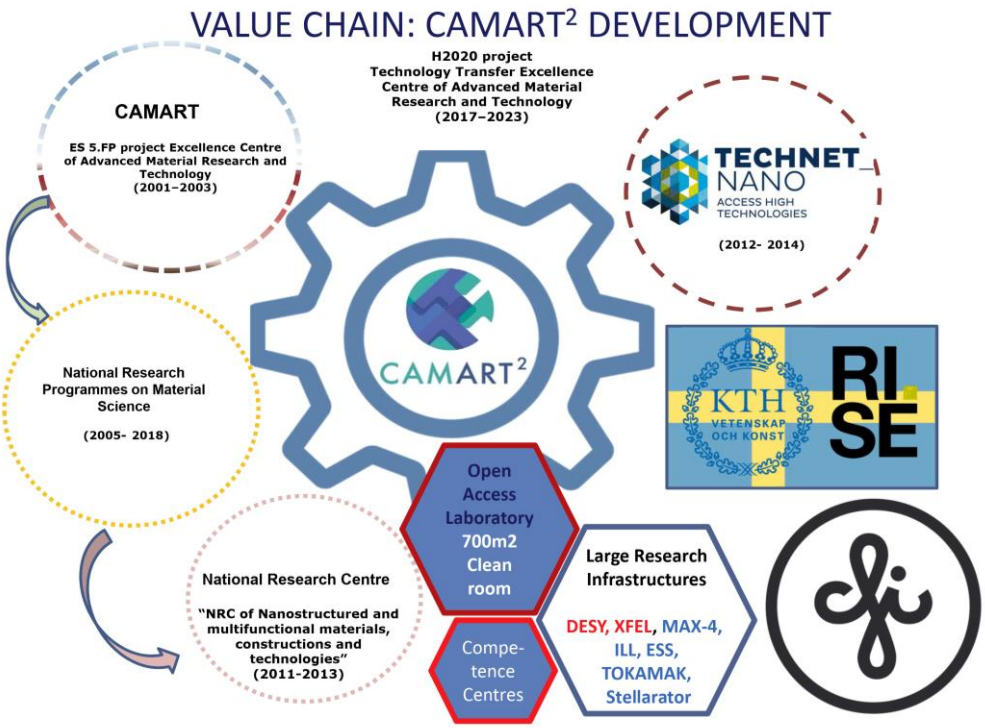


Figure 1: **Value chain: CAMART² development.**

ISSP UL has developed a strong research and innovation ecosystem that includes the following centers:

- Spectroscopy Centre;
- Nanotechnology Centre;
- Microscopy and Structure Analysis Centre;
- Thin Films Centre;
- Physical Chemistry (electrochemistry) Center;
- Computing Centre for Theoretical Modelling.

Complementary, ISSP UL is using possibilities offered by Large European Infrastructure centers such as synchrotron radiation facilities, incl. DESY PETRA-III and MaxIV Laboratory, EXFEL, and neutron spallation source - ESS. The ISSP UL work on in-situ studies of phase transitions was included in the MaxIV Highlights 2022.

In prototyping, ISSP UL specializes in using methods of optical and e-beam lithography, cleaning and surface preparation, dry etching, bonding and packaging, thermal processes, and wet chemistry.

Presently, ISSP UL is further focusing on education. An overhaul of the University's

master's and doctoral programs in physics and materials science is implemented. The ISSP UL's goal is to improve and enhance collaboration with industry in Latvia and abroad. To achieve this, a platform intended to serve as a single point of contact for scientists and companies has been established. Named Materize, the platform provides access to the ISSP UL's expertise and resources while also facilitating communication with companies to realise projects based on industry-specific standards. Current case studies being undertaken include a cleanroom-based prototyping facility, organic light-emitting diodes, optical lithography, vacuum deposition of thin films, and composite nanomaterials synthesis, material characterization, battery testing and coating development.

Every year the Innovation team of ISSP UL hosts events for idea creation, the Deep Science Hackathons. In 2023, the International hydrogen-themed hackathon "**Hydrogen X Future Hackathon**" took place on October, 6-8 at ISSP UL with 10 competing teams, and the Student Deep Science Hackathon took place on October, 20-22 with 14 competing teams. The Hackathon's goal was to identify high-tech ideas and find teams for their implementation, to create new products and companies that would contribute to the Baltic region's high-tech industry.

The Research Programme of ISSP UL for the period of 2021-2023-2027 includes the three thematic research areas of the Institute:

- Science: theory and experimental studies;
- Technology and experimental methods;
- Application: applied research of materials for sensors, scintillators, detectors, materials for photonics and electronics, and materials for energy harvesting and storage.

The Research Programme serves as an "entry-point" for advanced materials-related R&D&I challenges, inquiries, and proposals. It will help launch projects with a scope wider than that of a specific single research domain.

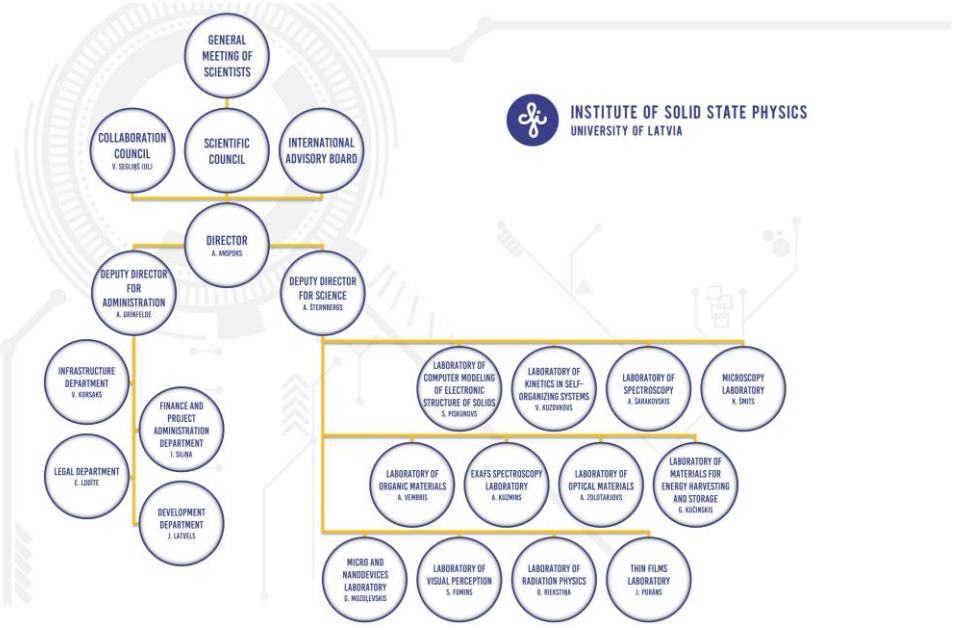
The long-term mission of the ISSP UL Research Programme 2021-2023-2027 and strategic development plan is to raise the Institute's scientific capacity and to integrate it better in the European Research Area.

In the year 2023, the domain concept continued to show positive results. 45 projects were implemented. They include Latvian Science Council Fundamental and Applied Research Projects (FARP): 18; Latvian National Research Program: 2 (NRP CERN, IF NRP "MOTE"); European Regional Development Fund (ERDF) projects: 5; Horizon Europe: 7; EUROfusion: 3;

COST projects: 1; M-EraNet: 5; Bilateral projects - Osmoze (France): 1 and Baltic- Norway: 1; LU fonds: 1; ESA RPP: 1.

The structure of ISSP UL at the end of 2023 is shown in Figure 2. It promotes research and innovation by creating a service-oriented environment, fostering openness and product-oriented research.

Figure 2: **The organizational structure of ISSP UL in 2023**



The highest decision-making body of ISSP UL is the **Scientific Council,** consisting of 15 members elected by the employees of the Institute (Table 1). Presently, Dr.phys. J. Butikova is the Acting Chair of the ISSP UL Scientific Council. The Council appoints the director and his/her deputies.

The Scientific Council of the Institute

1. Jeļena Butikova, Dr.phys., Acting Chair of the Scientific Council
2. Andris Anspoks, Dr.phys.
3. Dmitry Bocharov, Dr.phys.
4. Edgars Butanovs, Ph.D.
5. Līga Grīnberga, Dr.phys.
6. Aleksejs Kataševs Dr.phys., RTU.
7. Guntars Kitenbergs Dr.phys., UL.
8. Sergejs Piskunovs Dr.rer.nat.

9. Boriss Poļakovs Dr.phys.
10. Kaspars Pudžs Dr.phys.
11. Mārtiņš Rutkis, Dr.phys.
12. Anatolijs Šarakovskis, Dr.phys.
13. Andris Šternbergs, Dr.habil.phys.
14. Aivars Vembris, Dr.phys.
15. Virgīnija Vītola, Dr.phys.

To ensure an optimal alignment with global tendencies in material science, the ISSP UL performs consultations with the International Advisory Board when making strategic decisions. Additionally, the International Advisory Board issues recommendations for the commercialization of scientific results and for improving management.

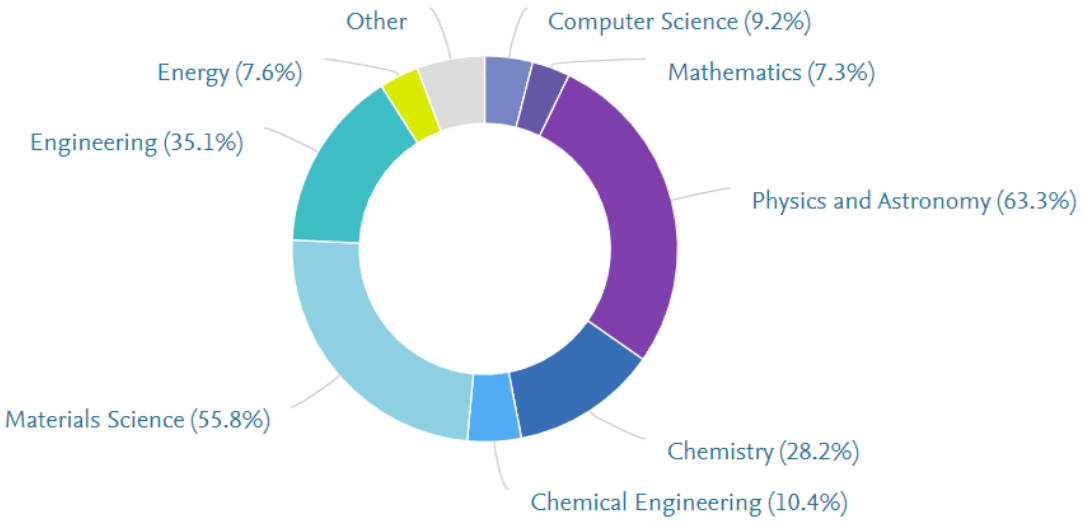
The International Advisory Board

1. Prof. Juras Banys, Vilnius University, Lithuania
2. Prof. Antonio Bianconi, Rome International Center for Materials Science Superstripes, Italy
3. Prof. Annette Bussmann-Holder, Max-Planck-Institute for Solid State Research, Germany
4. Prof. Ming-Chi Chou, Department of Materials and Optoelectronic Science, National Sun Yat-sen University, Taiwan, R.O.C.
5. Prof. Tony Donné, Programme Manager (CEO) for the consortium EUROfusion, the Netherlands
6. Prof. Dag Høvik, The Research Council of Norway, Norway
7. Prof. Marco Kirm, University of Tartu, Estonia
8. Prof. Maija Kuklja, Program director at National Science Foundation, USA
9. Dr. Jiri Kulda, Institut Laue-Langevin, France (IAB chairperson)
10. Dr. Nils Nordell, Director, Electrum Laboratory, KTH, Sweden
11. Prof. Toshio Ogawa, Shizuoka Institute of Science and Technology, Japan
12. Prof. Lars Österlund, The Ångström Laboratory, Uppsala University, Sweden
13. Dr. Mārtiņš Rutkis, Institute of Solid State Physics, University of Latvia, Latvia
14. Prof. Andrejs Silins, Latvian Academy of Sciences, Latvia
15. Dr.habil.phys. Andris Šternbergs, Institute of Solid State Physics, University of Latvia, Latvia
16. Prof. Pauls Stradins, Colorado School of Mines, USA

17. Honorary member Prof. Juris Upatnieks, Applied Optics, USA

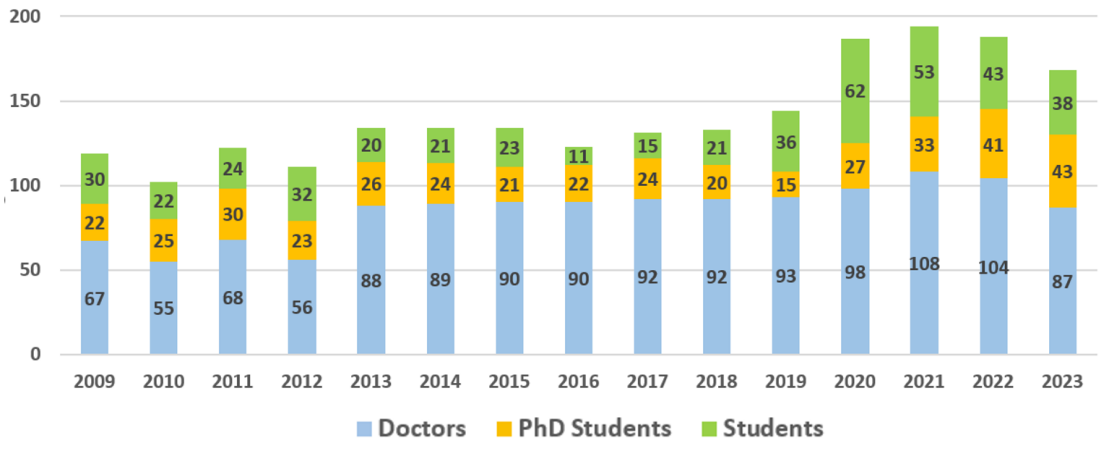
The multidisciplinary research (Figure 3) at the ISSP UL is performed by its highly qualified staff. On 31 December 2023, 244 employees were working at ISSP UL, including 87 researchers with PhD degrees and 5 administrative support staff members with PhD degrees. There were 43 PhD students, 19 MSc students, and 19 Bc students employed at ISSP UL in 2023. The total number of scientific staff was 138 including 68 Leading researchers, 33 researchers and 37 assistant researchers. Technical support staff number – 57, administrative staff – 49. The dynamics of the

Figure 3: Multidisciplinary research at ISSP UL: Publications by Subject Area



ISSP UL research staff is shown in Figure 4, indicating an impressive increase in the number of PhD students involved in the implementation of projects during the last two years. At the same time, a decrease in the number of Doctors is observed due to the natural generation change.

Figure 4: ISSP UL research staff dynamics 2009-2023



This Annual Report summarizes the research activities of the ISSP UL in 2023. The KPIs of ISSP UL are reported in Table 1.

Table 1:

Key performance indicators

Key performance indicators for Research	**3 years average (2015-2017)**	**2020**	**2021**	**2022**	**2023**	**2024 (Original end of CAMART² targets)**	**2026 (Sustainability targets)**
Number of scientific publications according to "Scopus"	119	127	122	195	**167**	333 (200)	400 (250)
A fraction of scientific publications in Int. Collaboration (%)	51	78	73	65	**72**	62	65
Number of citations/year according to "Scopus"	2043	3405	3082	3987	**3984**	3333	5000
Average SNIP per publication	0.79	0.95	1.04	0.96	**1.03**	1.15	1.25
Number of scientific and technical personnel (FTE)	105	138	141	153	**126**	173	175
Publications/FTE	1.13	0.92	0.87	1.27	**1.33**	1.91 (1.26)	2.29 (1.45)
Gender balance of scientific and technical personnel (% female)	26	30	31	31	**34**	37	40

In 2023, a total of 167 papers were published in peer-reviewed journals (5 papers are in press). 89 of them (54%) were published in journals with the SNIP factor >1 (48% in 2022). 86% of publications are in journals belonging to the Q1 and Q2 quartiles (compared to 85% in

2022).

It is necessary to separately note the publication in the high-impact journal (IF=22.1) - *Applied Catalysis B: Environmental* (DOI: 10.1016/j.apcatb.2022.122183). This comprehensive study was performed in collaboration with the teams from the Department of Chemical Engineering, National Taiwan University (Taipei, Taiwan) and the Advanced Materials Department, Jožef Stefan Institute (Ljubljana, Slovenia) with a prominent contribution from the ISSP UL team. It was demonstrated that the twin photoreactor, utilizing a core-shell structural Rh-CrO_x loaded on Al^{3+}-doped strontium titanate, can, simultaneously, generate pure hydrogen and degrade isopropanol thus having a high potential for hydrogen production from water splitting by sunlight harvesting.

Several metrics as provided by the SCOPUS database were used to evaluate the research output of ISSP UL and its change during the last eight years (2016-2023). They were calculated using the SciVal research performance assessment tool, which allows analysis of the data from Scopus.

The first two metrics indicate how many ISSP UL publications are among the most-cited ones within the entire Scopus database or have been published in the most-cited journals indexed by Scopus. The percent of ISSP UL publications that are among the top 10% of most cited publications worldwide was 18% in 2023 (12% in 2022) (Figure 5). The percent of publications in the top 10% of the most-cited journals indexed by Scopus was maintained at 22% in 2023 (18% in 2022) (Figure 6).

Figure 5: Percentage of ISSP UL publications that fall within the top 10% of the most cited worldwide publications (from Scopus database)

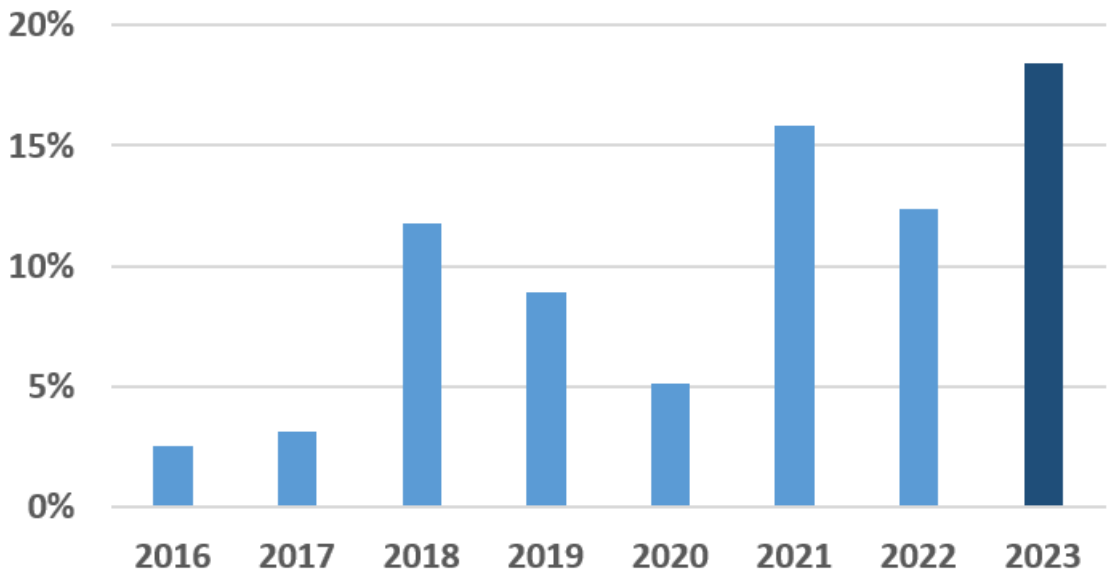
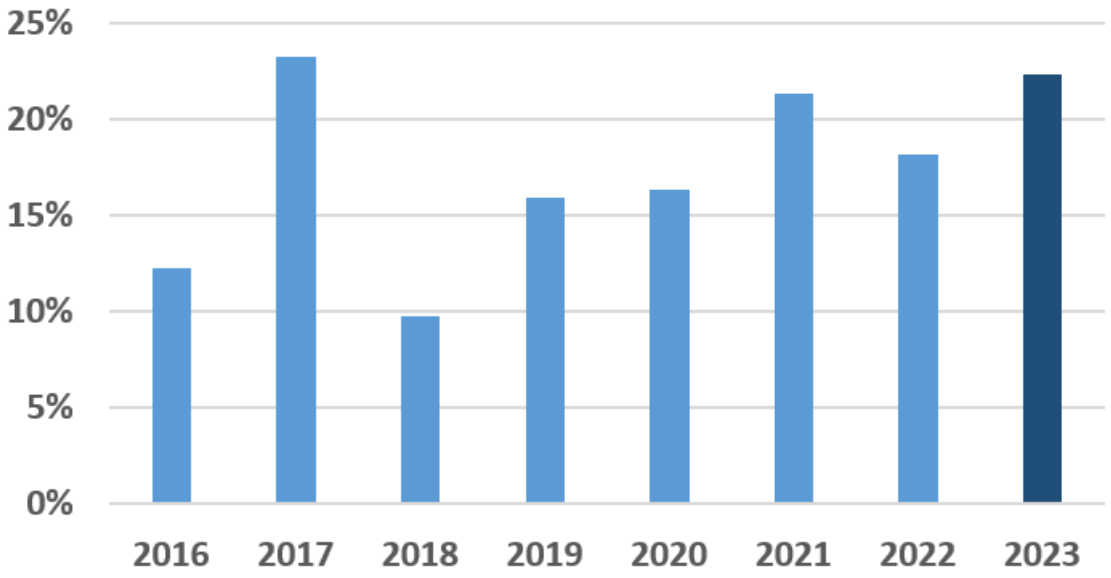


Figure 6: Share of the ISSP UL publications belonging to the top 10% of the most-cited journals indexed by Scopus (from Scopus database)



The third metric, Field-Weighted Citation Impact (FWCI), measures how citations received by ISSP UL publications compare to the world average. An FWCI value of 1.00 indicates that the entity's publications were cited exactly as one would expect based on the global average of similar publications. The FWCI of ISSP UL publications was 0.87 in 2022 and 0.88 in 2023, thus indicating high publication quality and stability (Figure 7).

The fourth metric shows the distribution of ISSP UL publications across journals, divided into four quartiles according to their Impact Factor. It is important to stress that about 86% (85% in 2022) of all publications in 2023 appeared in journals belonging to the first (Q1) and second (Q2) quartile (Figure 8).

Building the research capacity and development of human capital are among the priorities at ISSP. These are addressed in collaboration with the University of Latvia and other universities through the preparation of the next generation of researchers. The ISSP is a traditional place where many students start and accelerate their research careers to Bachelor's, Master and PhD levels. In 2023, 4 PhD, 7 MSc, and 7 Bc theses were prepared and successfully defended.

Figure 7: Field-Weighted Citation Impact (FWCI) of ISSP UL publications compared with the world average. A FWCI of 1.00 indicates that the ISSP UL publications have been cited exactly as would be expected based on the global average for similar publications (from Scopus database)

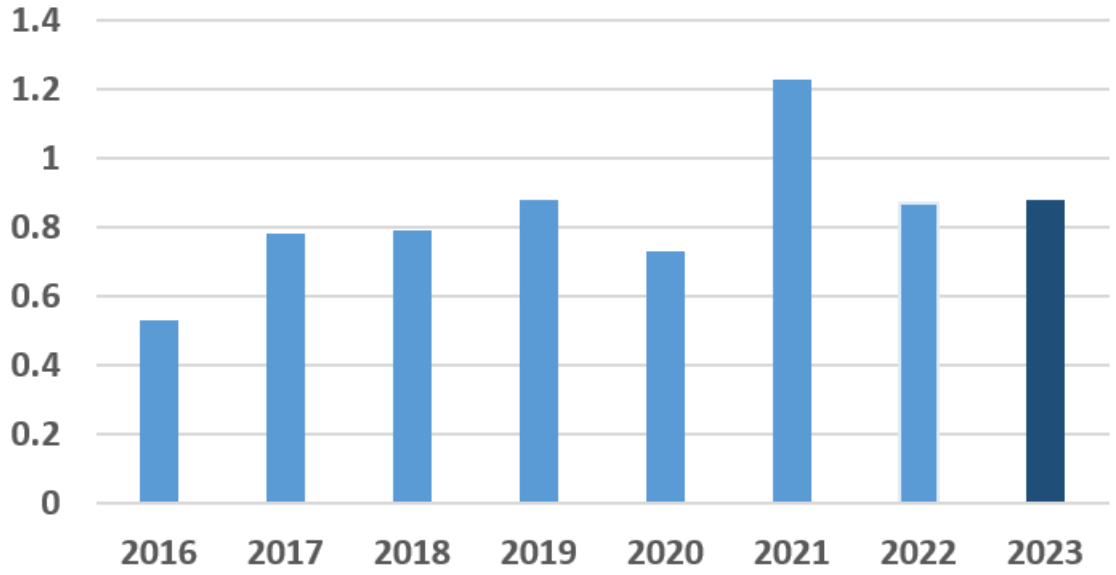
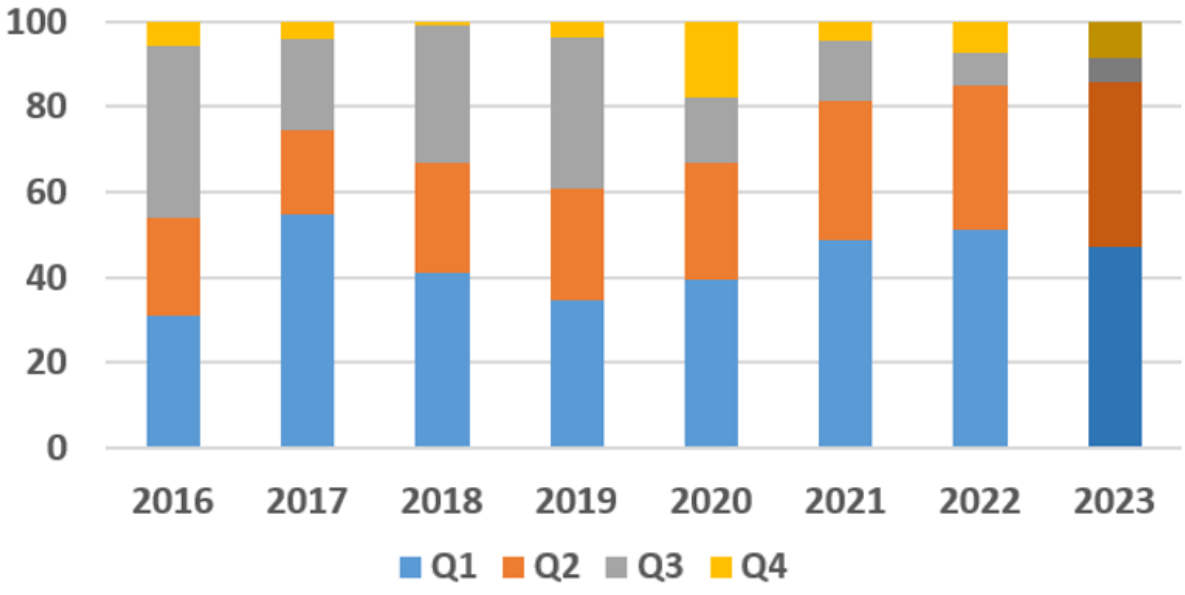


Figure 8: ISSP UL publications by Journal quartile (from Scopus database)

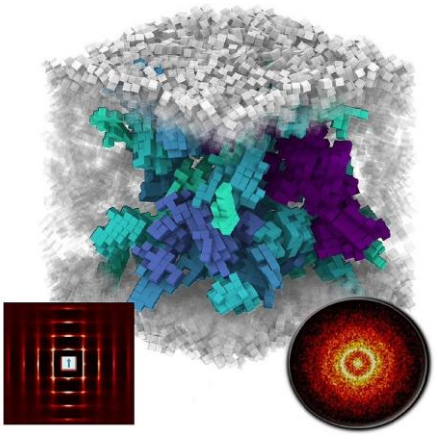


The high quality of the research at ISSP UL was recognized at the international and national levels. Doctoral student M.sc.ing. Katrīna Laganovska received the L'Oréal-UNESCO Baltic for Women in Science award for a project on the study of optical properties and defects in ferroelectric metal oxides. Two studies conducted by the ISSP UL teams were among the

winners of the Science Achievements Competition 2023 by the Latvian Academy of Sciences (LAS). The first study on “Computer design of perovskite nanoparticles for efficient hydrogen production” (Dr. Hab phys. E.Kotomin, et.al) was entirely implemented at ISSP UL, whereas the second study on "Novel materials for development of all-optical temperature sensor" (U.Rogulis, et.al) was conducted in collaboration between ISSP UL and Light Guide Optics International (Livani, Latvia). The main annual Latvenergo and Latvian Academy of Sciences award named after Professor A. Vītols for outstanding contribution to energetics was received by Dr.chem. Gunārs Bajars for outstanding contribution "Materials research for electrochemical energy storage in batteries and accumulators". Annual awards also went to two young scientists: Dr. phys. Gints Kučinskis for his doctoral thesis "Research of cathode materials for sodium-ion batteries" and Dr. phys. Mārtiņš Zubkins for his doctoral thesis "New coatings based on metal hydride and oxide for energy, electronics and health care technologies".

Scientific Highlights

I. Science: Theory and experimental studies



Efficient ultrafast laser writing with elliptical polarization

Yuhao Lei[1], Gholamreza Shayeganrad[1], Huijun Wang[1], Masaaki Sakakura[1], Yanhao Yu[1], Lei Wang[1], Dmitrii Kliukin[1], Linards Skuja[2], Yuri Svirko[3], Peter G. Kazansky[1]

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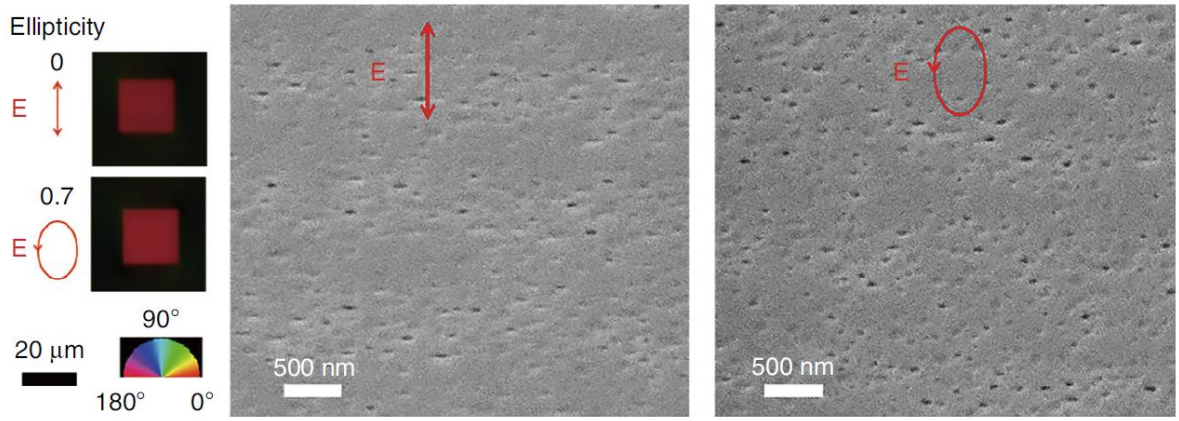
[2] Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., Riga LV-1063, Latvia.
[3] Institute of Photonics, Department of Physics and Mathematics, University of Eastern Finland, FI-80101 Joensuu, Finland

Photosensitivity in nature is commonly associated with stronger light absorption. It is also believed that artificial optical anisotropy is the strongest when created by light with linear polarization. Contrary to common belief, the maximum induced birefringence occurs at an ellipticity of 0.6 and not at linear polarization. This is a consequence of the balance between the concentration of nanopores with a maximum at circular polarization and their shaping due to the anisotropy of the near-field enhancement produced by the linear polarization component. It is suggested that enhanced interaction of a circularly polarized beam with randomly oriented bonds and activation of self-trapped holes in silica glass, as well as more efficient tunneling ionization of defects with low excitation energy by circular polarization are responsible for this phenomenon. In addition, the voltage required to control the elliptical polarization is significantly reduced, which allows the use of electro-optical modulators with higher modulation frequency for birefringence patterning. Writing with elliptically polarized laser pulses makes it possible to reduce the pulse energy and increase the recording speed in 5D optical data storage, as well as reduce the manufacturing time of geometric phase optical elements.



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Y. Lei, G. Shayeganrad, H. Wang, M. Sakakura, Y. Yu, L. Wang, D. Kliukin, L. Skuja, Y. Svirko, P. G. Kazansky, Light: Science & Applications 12 (2023) 74. DOI: 10.1038/s41377-023-01098-2.

Proton migration barriers in $BaFeO_{3-\delta}$ – insights from DFT calculations

M. F. Hoed[1], A. Chesnokov[2], D. Gryaznov[2], R. Merkle[1], E. A. Kotomin[1,2], J. Maier[1]

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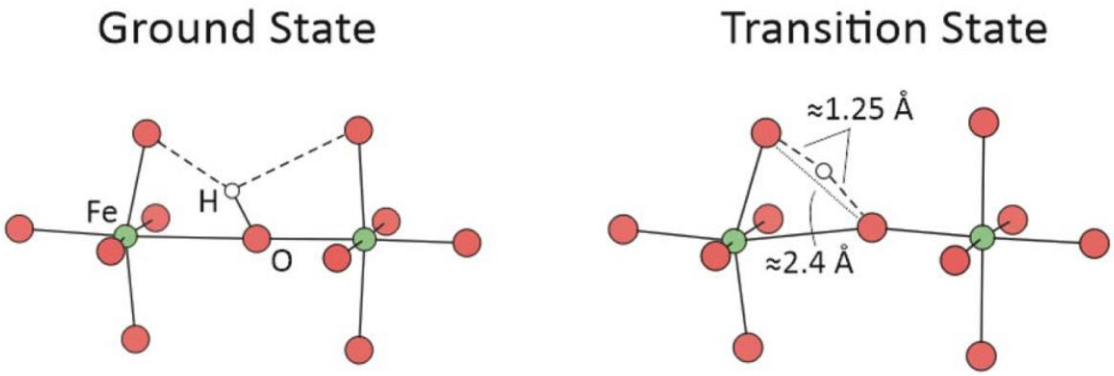
[2] Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., Riga LV-1063, Latvia.
[3] Institute of Photonics, Department of Physics and Mathematics, University of Eastern Finland, FI-80101 Joensuu, Finland

Proton migration in the triple conducting perovskite $BaFeO_{3-\delta}$ is investigated using first-principles density functional theory calculations. Oxygen-deficient $BaFeO_{3-\delta}$ exhibits pronounced lattice distortions that entail different chemical environments of lattice oxygen ions and thus different proton migration pathways.

In this study, we systematically sampled these proton pathways and identified key structural parameters determining the height of the migration barrier. The calculated average migration barrier for proton transfer in Jahn–Teller distorted $BaFeO_3$ is 0.22 eV. Analysis of geometric changes and chemical bonding in individual proton trajectories indicates that proton transfer occurs as a two-step process: an early stage where the energy change is mainly governed by the approach of donor and acceptor oxygen ions (the O–H bond is hardly stretched), and a second stage near the transition state where the O–H bond is broken. The calculated average migration barrier in oxygen-deficient $BaFeO_{2.75}$ is 0.18 eV, with a broad range of different barriers due to the increased lattice distortions caused by oxygen vacancies. The decrease in migration barrier with increasing oxygen deficiency could be attributed to the annihilation of oxygen (ligand) holes rather than to volume expansion upon reduction. Considering all calculated barriers in $BaFeO_3$ and $BaFeO_{2.75}$ we find important correlations of the migration barrier height with the initial separation of donor and acceptor oxygen ions, and the O–H bond length. While this co-dependence reflects the two-step nature of proton transfer, it is also helpful for the optimization of triple-conducting oxides for various electrochemical applications.



Published in:
M. F. Hoed, A. Chesnokov, D. Gryaznov, R. Merkle, E. A. Kotomin, J. Maier, J. Mater. Chem. A 11 (2023) 6336–6348. DOI: 10.1039/d2ta08664f.

Local structure and magnetic properties of a nanocrystalline Mn-rich Cantor alloy thin film down to the atomic scale

A.Smekhova[1], A. Kuzmin[2], K. Siemensmeyer[1], C. Luo[1,2], J. Taylor[1,2], S. Thakur[4], F. Radu[1], E. Weschke[1], A. Guilherme Buzanich[5], B. Xiao[6], A. Savan[6], K. V. Yusenko[5], A. Ludwig[6]

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[2] *Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., Riga LV-1063, Latvia.*
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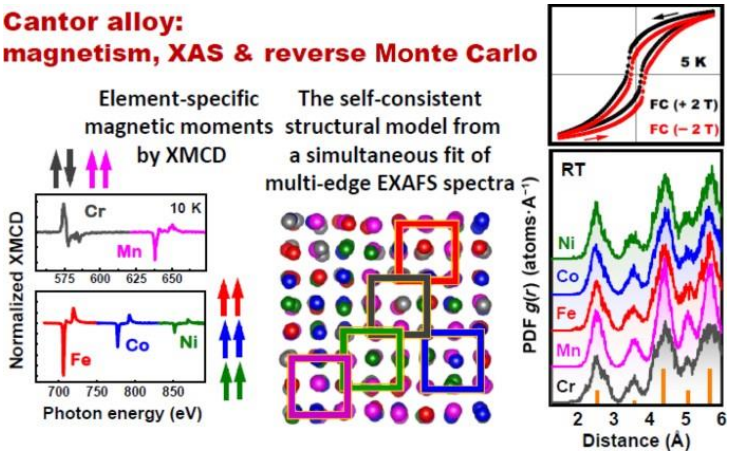
[5] *Bundesanstalt für Materialforschung und-prüfung (BAM), Berlin, D-12489, Germany*
[6] *Institut für Werkstoffe, Ruhr-Universität Bochum, Bochum, D-44801, Germany*

The huge atomic heterogeneity of high-entropy materials along with the possibility to unravel the behavior of individual components at the atomic scale suggests a great promise in designing new compositionally complex systems with the desired multi-functionality. Herein, we apply multi-edge X-ray absorption spectroscopy (EXAFS/XANES), and X-ray magnetic circular dichroism (XMCD)) to probe the structural, electronic, and magnetic properties of all individual constituents in the single-phase face-centered cubic (fcc)-structured nanocrystalline thin film of Cr20Mn26Fe18Co19Ni17 (at.%) high-entropy alloy on the local scale. The local crystallographic ordering and component-dependent lattice displacements were explored within the reverse Monte Carlo approach applied to EXAFS spectra collected at the K absorption edges of several constituents at room temperature. A homogeneous short-range fcc atomic environment around the absorbers of each type with very similar statistically averaged interatomic distances (2.54–2.55 Å) to their nearest-neighbors and enlarged structural relaxations of Cr atoms were revealed. XANES and XMCD spectra collected at the $L_{2,3}$ absorption edges of all principal components at low temperature from the oxidized and in situ cleaned surfaces were used to probe the oxidation states, the changes in the electronic structure, and magnetic behavior of all constituents at the surface and in the sub-surface volume of the film. The spin and orbital magnetic moments of Fe, Co, and Ni components were quantitatively evaluated. The presence of magnetic phase transitions and the co-existence of different magnetic phases were uncovered by conventional magnetometry in a broad temperature range.



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A. Smekhova, A. Kuzmin, K. Siemensmeyer, C. Luo, J. Taylor, S. Thakur, F. Radu, E. Weschke, A. Guilherme Buzanich, B. Xiao, A. Savan, K. V. Yusenko, A. Ludwig, Nano Res. 16 (2023) 5626–5639. DOI: 10.1007/s12274-022-5135-3.

Paramagnetic Point Defect in Fluorine-Doped Silica Glass: The E’ (F) Center

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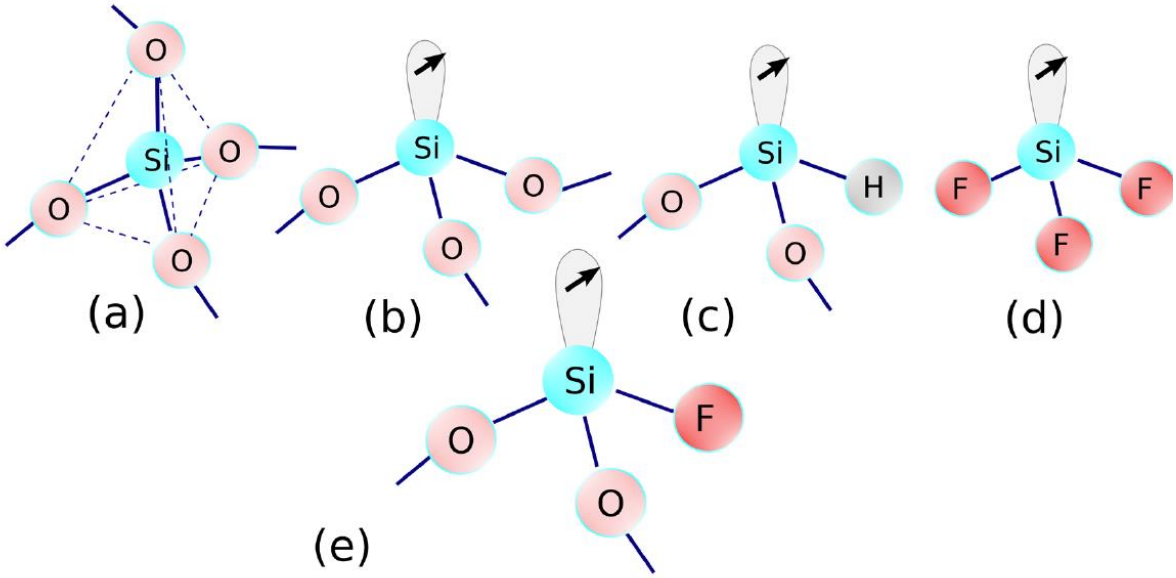
Fluorine-doped silica is a key material used in all low-loss and/or radiation-resistant optical fibers. Surprisingly, no fluorine-related radiation-induced point defects have been identified. By using electron paramagnetic resonance, we report the first observation of F-related defects in silica. Their fingerprint is a doublet with 10.5 mT splitting due to hyperfine coupling (hfc) to ^{19}F nuclear spins. An additional 44.4 mT hfc to the ^{29}Si nucleus indicates that this defect belongs to the “E’ center” family and has a structure of a fluorine-modified Si dangling bond: 3-coordinated Si atoms with an unpaired electron in an sp3 orbital, bonded to a glass network by 2 bridging oxygen atoms and to a F atom.



Regular SiO_4 tetrahedron (a) in silica glass network and structures of paramagnetic dangling Si bond centers: generic E’ center (b), H(I) center (c), SiF_3 radical (d), and the proposed structure of E’(F) center (e).

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Critical review on experimental and theoretical studies of elastic properties of wurtzite-structured ZnO nanowires

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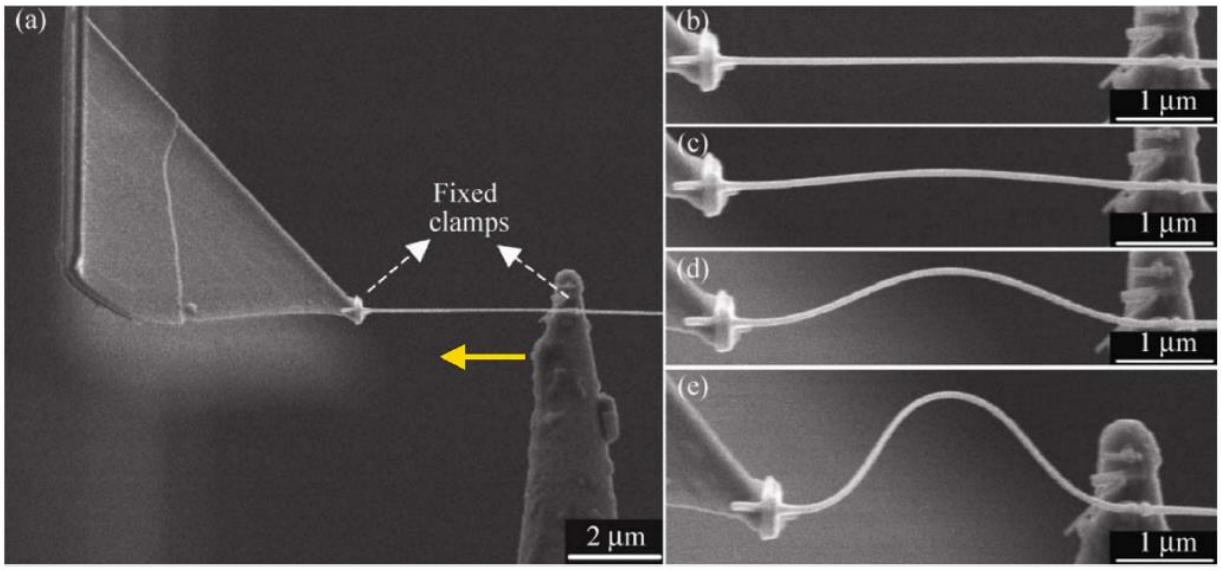
In this critical review, we call attention to a widespread problem related to the vast disagreement in elastic moduli values reported by different authors for nanostructures made of the same material. As a particular example, we focus on ZnO nanowires (NWs), which are among the most intensively studied nanomaterials due to their remarkable physical properties and promising applications. Since ZnO NWs possess piezoelectric effects, many applications involve mechanical deformations. Therefore, there are plenty of works dedicated to the mechanical characterization of ZnO NWs using various experimental and computational techniques. Although the most of works consider the same growth direction and wurtzite crystal structure, reported values of Young's modulus vary drastically from author to author ranging from 20 to 800 GPa. Moreover, both – diameter-dependent and independent – Young's modulus values have been reported. In this work, we give a critical overview and perform a thorough analysis of the available experimental and theoretical works on the mechanical characterization of ZnO NWs to find out the most significant sources of errors and to bring out the most trustable results.



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Effect of ‘in-plane’ contraction on the (001) surface of the model perovskite $SrTiO_3$

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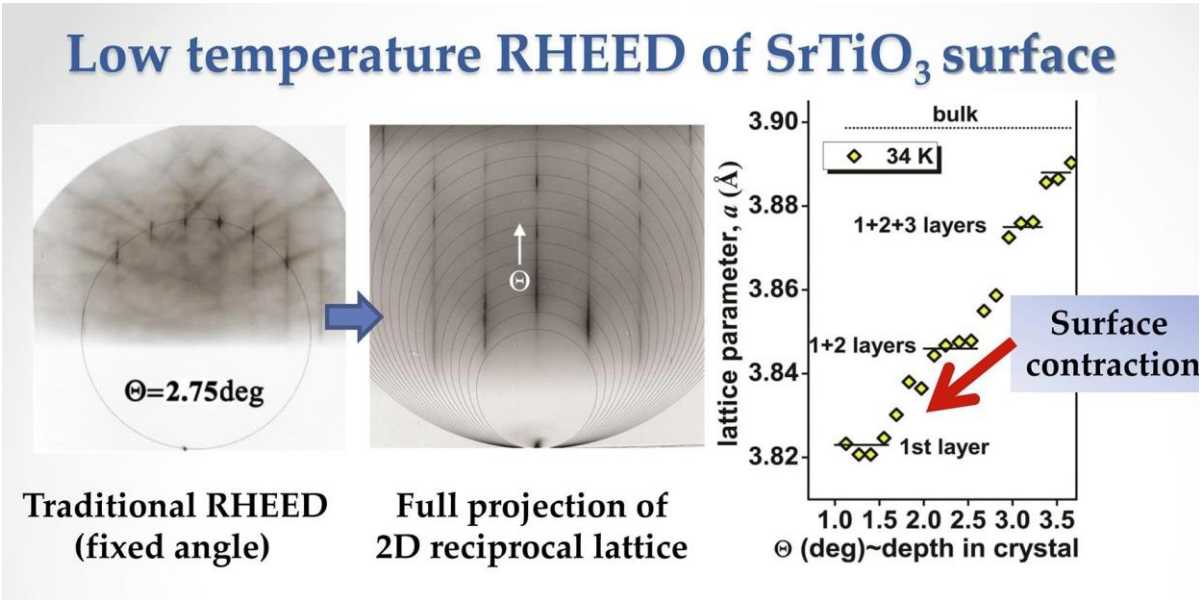
Reflection high-energy electron diffraction in the temperature range 8–300 K revealed several surface structural transformations accompanied by a strong ‘in-plane’ lattice parameter growth on the (001) surface of the model perovskite $SrTiO_3$ single crystal. Rather may occurring at sharp temperatures, these transformations are observed to extend over temperature intervals separated from each other by temperature zones, where no structural changes occur, and the crystal lattice is relaxed. In such relaxed zones, the equilibrium lattice parameters were identified and analyzed as a function of penetration depth. A strong ‘in-plane’ contraction of the crystal lattice in the first surface layers was experimentally revealed at low temperatures and theoretically confirmed by hybrid DFT calculations. Along with such an ‘in-plane’ contraction of the (001) surface at low temperatures, we have found that the thermal expansion on the surface is much higher than in the bulk which results in approaching the surface ‘in-plane’ and the bulk lattice parameters at room temperature. This contradicts the general assumption that surface ‘in-plane’ and bulk lattice parameters are identical.



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Reasonable BN nanotubes composed of B–B and N–N bonds: A theoretical prediction

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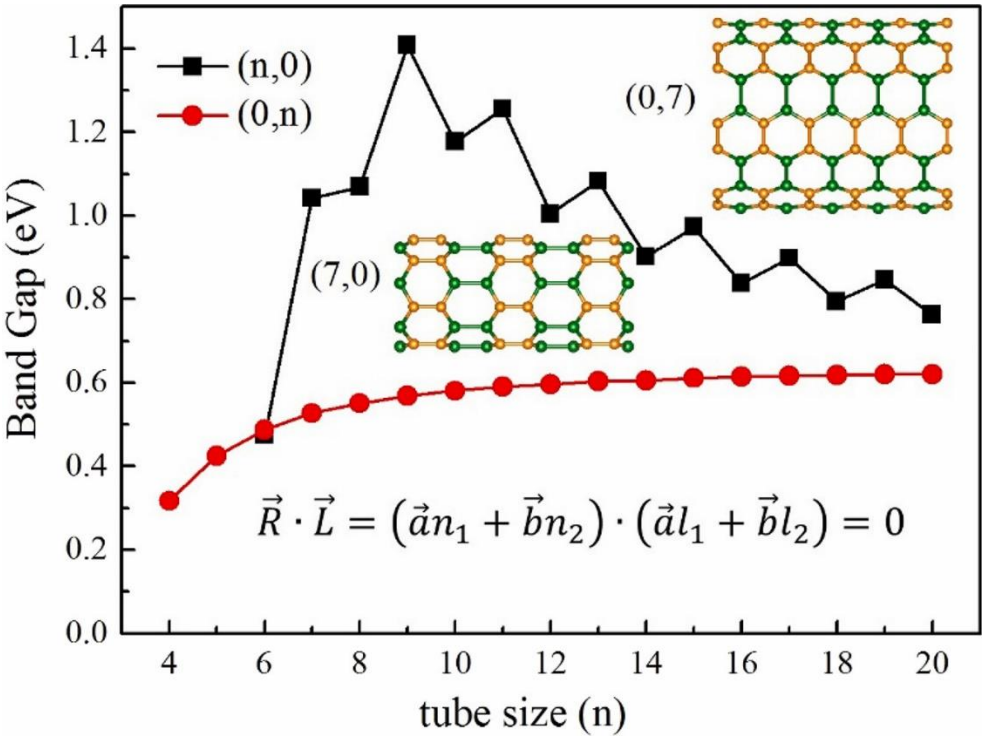
A nanotube is one of the most important one-dimensional (1D) materials at the nanoscale. The most famous family among them is the carbon nanotubes. What kinds of nanotubes rolled from the rectangular di-BN are indeed reasonable? In order to clarify this question, two types of mathematically and physically rigorous boron nitride nanotubes (di-BNNTs) along the (n, 0) and (0, n) chiral vectors, composed of diboron B−B and azo N−N bonds, are investigated with the aid of density functional theory (DFT) simulations. Firstly, there is no chiral nanotube with (n, m) at all by considering its 1D periodicity. Secondly, the phonon dispersion relations clearly support the lattice dynamic stabilities of the thinnest zigzag (6, 0) and armchair (0, 4) di-BNNTs with radii of 2.385 Å and 2.911 Å, respectively. The ab-initio molecular dynamics (AIMD) simulations further confirm their thermodynamic stabilities at least at 1000 K. Furthermore, the energetic, mechanical, and electronic features of these two kinds of di-BNNTs are systematically studied. According to our calculations, di-BNNTs possess excellent mechanical strengths and adjustable band gaps, which endow them the promising application potential in the solar conversion field.



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DOI: 10.1016/j.apsusc.2022.155156.

Doping at sp^3-site in Me-graphene (C568) for new anodes in rechargeable Li-ion battery

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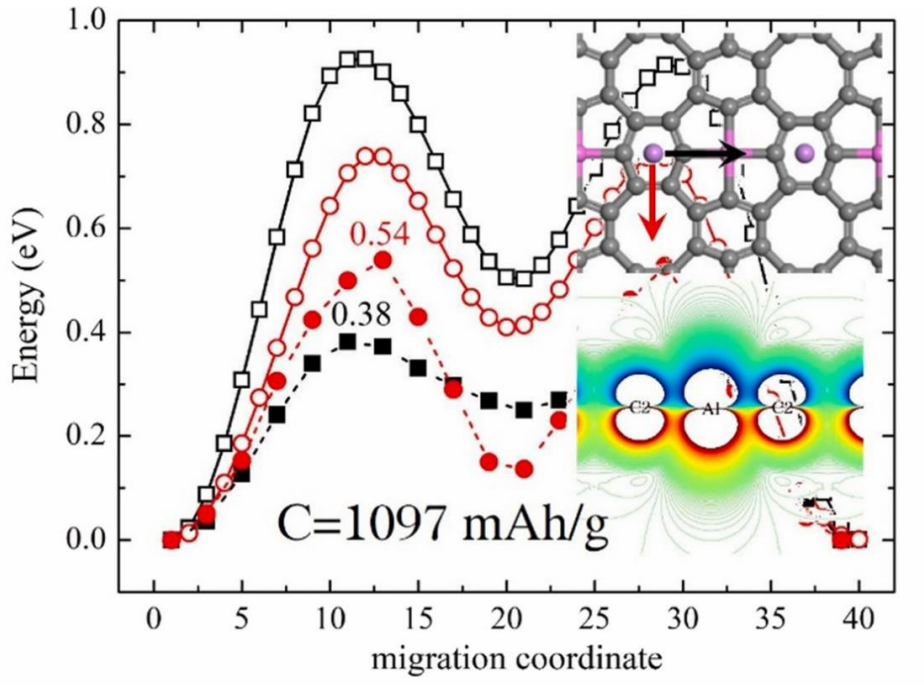
In the last two decades, low-dimensional materials, especially the low-dimensional carbon allotropes, gained a substantial amount of attention from both academia and industry owing to their unique mechanical and electronic features. In this theoretical study, the monolayer carbon allotrope, Me-graphene (also called C568), was respectively doped with Al, Si, P, and Ge atoms by substituting the sp^3-hybridized carbon atom in its unit cell to manipulate its physical properties. Theoretical calculations based on the density functional theory (DFT) confirmed the dynamic stabilities of the related doping systems. Interestingly, the mechanical strengths of the doping systems are even stronger than the pristine ones. After doping with the Si atom, the band gap of the Me-graphene system narrowed from 1.097 eV to 0.987 eV estimated at the HSE06 level. However, the Ge-dopant at the -site has very limited influence on the band gap. In the other two cases with Al and P dopants, the systems changed to metallic because their Fermi levels cut into the valence bands to a certain extent. Additionally, the adsorption sites of Li atoms and the energy profiles of the Li migrations on the related 2D material systems were also investigated in order to reveal their application potentials as anodes in lithium-ion batteries (LIBs).



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W.-H. Zhao, F.-Y. Li, H.-X. Zhang, R. I. Eglitis, J. Wang, R. Jia, Applied Surface Science 607 (2023) 154895.
DOI: 10.1016/j.apsusc.2022.154895.

Dielectric behaviour of nitrogen doped perovskite $SrTiO_{3-\delta}N_{\delta}$ films

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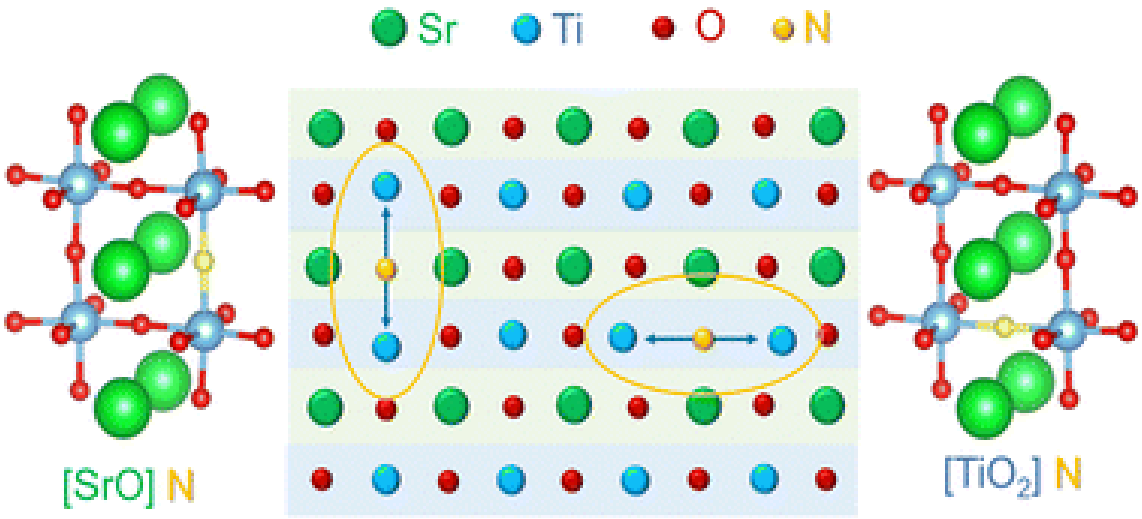
Technologically important high-permittivity dielectrics are often achieved using cationic engineering of ABO_3-type perovskite para(ferro)electrics. Here, we experimentally and theoretically explore the potential of less conventional anionic engineering in ABO_3 dielectrics. We demonstrate that in an archetypal representative $SrTiO_3$, nitrogen substitution can occur on two distinct oxygen atomic sites, reduce crystal symmetry, and lead to significant changes in the patterns and frequencies of lattice vibrations. These phonon transformations diminish permittivity, whereas contribution from nitrogen-induced nanoregions can raise it. The effects of nitrogen are found to be especially strong in epitaxial films. The unveiled mechanism for the nitrogen-controlled dielectric constant through increased complexity of the lattice vibrations may be akin to many technologically important perovskite oxide para(ferro)electrics.



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Band Gap Regulation with Imino Groups in Graphdiyne: A Promising Photocatalyst for Water-Splitting and CO_2 Reduction

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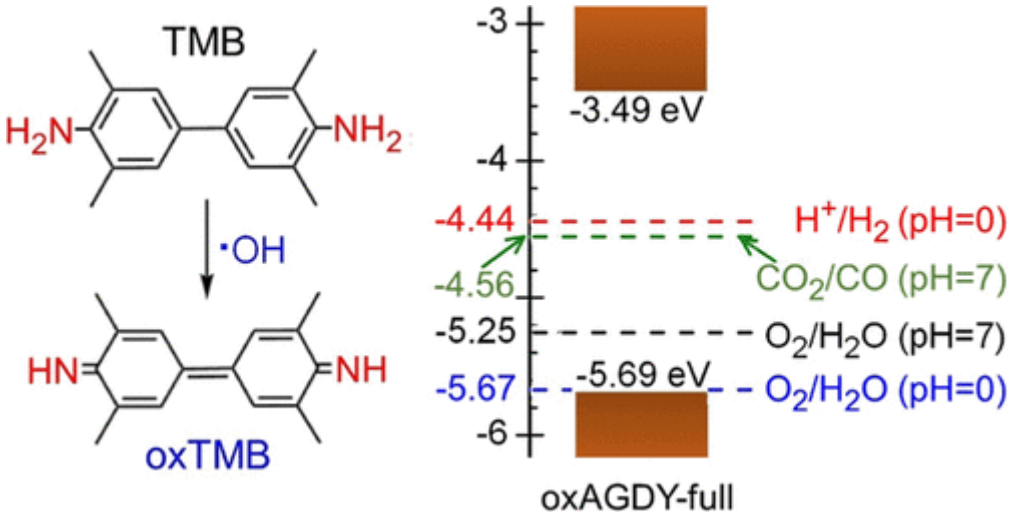
In this work, two-dimensional (2D) GDY derivatives with the imino groups were investigated with the aid of density functional theory (DFT) calculations. Their structural stabilities were carefully verified. The geometric configurations and mechanical properties of the related systems as well as some typical reference systems were introduced and discussed. At the G_0W_0 level, the band gaps of the related systems with imino groups are in the range of 1.50–2.20 eV, which are optimal for visible light absorption. Their band edges are more dispersive than those in the other existing GDY derivatives (e.g., F-, H-, and CN-GDYs), leading to their outstanding charge carrier mobilities. Moreover, their band edge arrangements imply the photocatalytic abilities for the complete water-splitting reaction and CO_2 reduction. The substitution with imino groups is an effective way to enhance the solar energy harvesting efficiency of the GDY system and its derivatives.



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J.-Q. Zhang, B. Hu, A. Dong, R.I. Eglitis, Z.-J. Yi, R. Jia, ACS Applied Nano Materials 6 (23) (2023) 22506-22516. DOI: 10.1021/acsanm.3c05354.

Thermostimulated luminescence analysis of oxygen vacancies in HfO_2 nanoparticles

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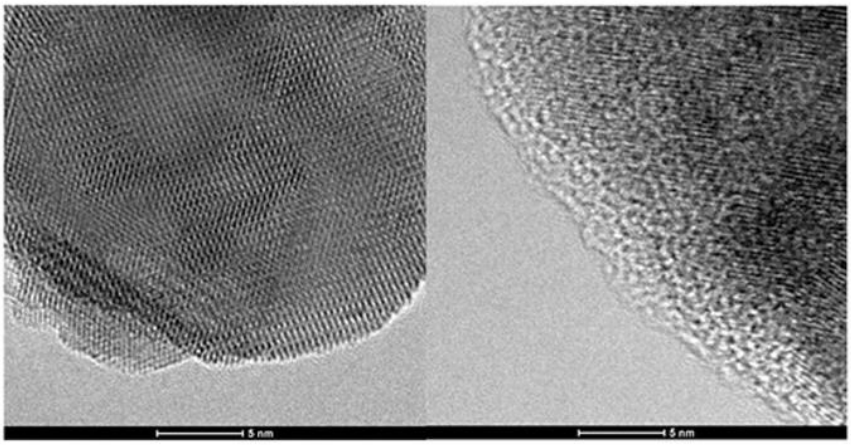
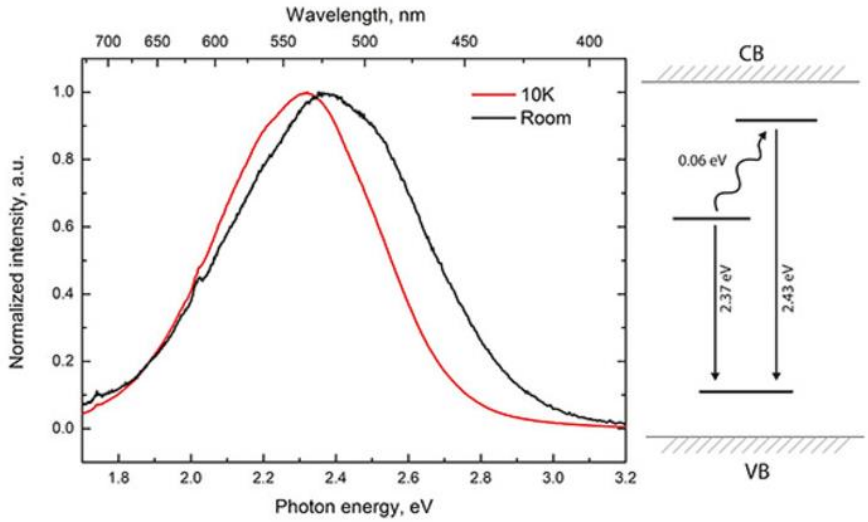
Institute of Solid State Physics, University of Latvia, Kengaraga Street 8, LV-1063 Riga, Latvia

Hafnia has already been established in CMOS technologies as a high-k metal gate material, however, recently it has also become a promising material in ferroelectric applications. In this study, we have investigated intrinsic defects such as oxygen vacancies in undoped and 5at%Eu HfO_2 synthesized by sol-gel, combustion, auto-ignition combustion, hydrothermal and precipitation methods. All samples were of monoclinic phase with crystallite sizes of 16–40 nm. Photoluminescence (PL) and thermostimulated luminescence (TSL) both below and above room temperature as well as XRD and TEM methods were used to identify potential VO_3^{+1}, VO_3^{+2}, VO_4^{+1} and VO_4^{+2} defects. Activation energies were determined for the oxygen vacancies and grain boundary effects were studied. Both PL and TSL wavelength peak spectra shift to higher energies with the increase in temperature.





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Ir impurities in α- and β-Ga_2O_3 and their detrimental effect on p-type conductivity

A. Zachinskis[1], J. Grechenkov[1], E. Butanovs[1], A. Platonenko[1], S. Piskunov[1], A.I. Popov[1], J. Purans[1], D. Bocharov[1,2]

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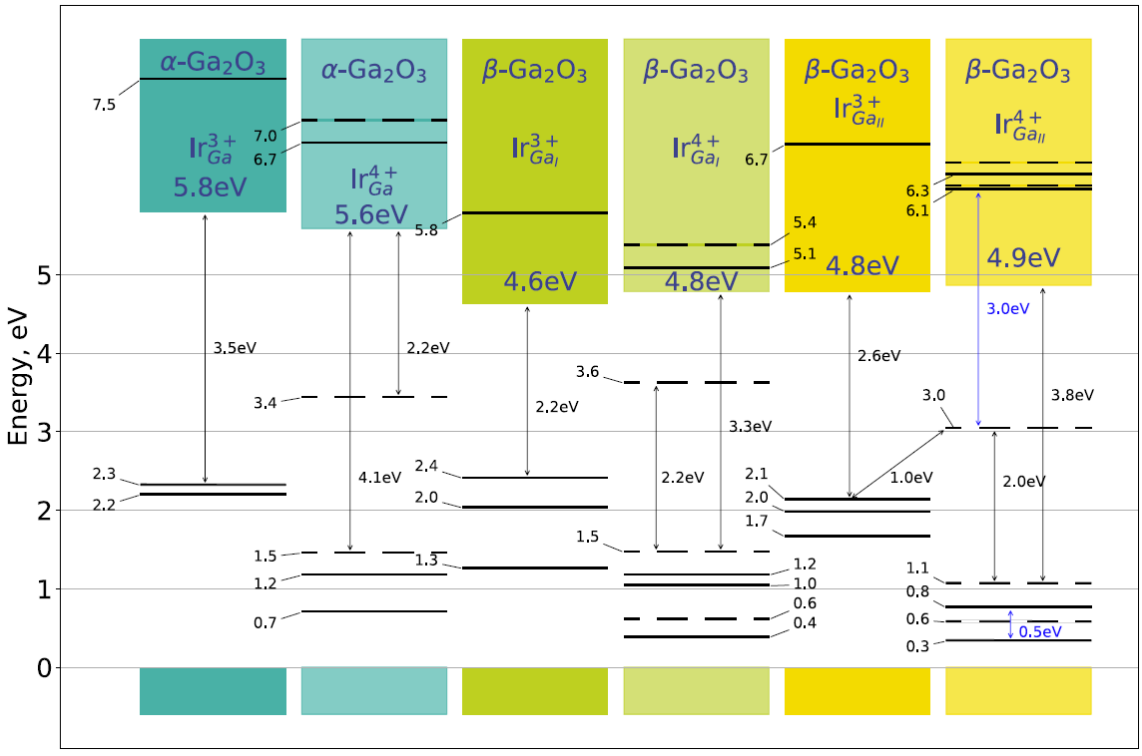
Recently gallium oxide (Ga_2O_3) has become one of the most actively studied materials due to its competitive electronic properties such as wide bandgap, high breakdown field, simple control of carrier concentration, and high thermal stability. These properties make gallium oxide a promising candidate for potential applications in high-power electronic devices. β-Ga_2O_3 crystals are commonly grown by the Czochralski method in an iridium (Ir) crucible. For this reason, Ir is often present in crystals as an unintentional dopant. In this work the impact of Ir incorporation defects on potential p-type conductivity in β-Ga_2O_3 is studied by means of density functional theory. The metastable α-Ga_2O_3 phase was investigated as the model object to understand the processes caused by iridium doping in gallium oxide-based systems. Obtained results allow us to understand better the influence of Ir on electronic structure, as well as provide interpretation for optical transitions reported in recent experiments.



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A. Zachinskis, J. Grechenkov, E. Butanovs, A. Platonenko, S. Piskunov, A.I. Popov, J. Purans, D. Bocharov, Scientific Reports 13 (2023) 8522. DOI: 10.1038/s41598-023-35112-9.

Jahn–Teller distortion in Sr_2FeO_4: group-theoretical analysis and hybrid DFT calculations

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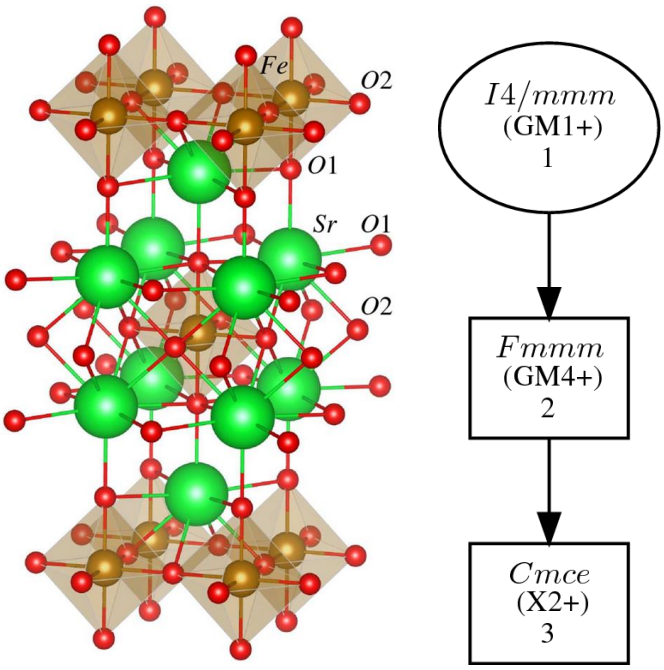
Discovered in the 1950s in pioneering works for perovskite $SrTiO_3$ structures, i.e. Sr_2TiO_4 and $Sr_3Ti_2O_7$, materials able to exist in the Ruddlesden–Popper (RP) structure (ABO) are experiencing growing interest due to high technological relevance. An intriguing interplay between behaviours of perovskite (ABO) and rock salt (AO) layers (phases) in the RP structure lies at the heart of this growing interest.

We present theoretical justification for distorted Ruddlesden–Popper (RP) phases of the first-order by using hybrid density functional theory (DFT) calculations and group-theoretical analysis. We, thus, demonstrate the existence of the Jahn–Teller effect around a Fe^{4+} ion in Sr_2FeO_4. On the calculation side, we have established a combination of Wu–Cohen (WC) exchange and Perdew-Wang (PW) correlation in a three-parameter functional WC3PW, giving the most accurate description of Sr_2FeO_4 from the comparison of three hybrid DFT functionals. Self-consistently obtained Hartree–Fock exact exchange of 0.16 demonstrates consistent results with the experimental literature data. Importantly, we explain conditions for co-existing proper and pseudo-Jahn–Teller effects from the crystalline orbitals, symmetry-mode analysis and irreps products. Moreover, phonon frequency calculations support and confirm the results of symmetry-mode analysis. In particular, the symmetry-mode analysis identifies a dominating irreducible representation of the Jahn-Teller mode (X2+) and corresponding space group (SG) of ground state structure (SG Cmce model). Therefore, the usually suggested high-symmetry tetragonal crystal structure (SG I4/mmm model) is higher in energy by 121 meV/f.u. (equivalent to the Jahn-Teller stabilization energy) compared with the distorted low-symmetry structure (SG Cmce model). We also present diffraction patterns for the two crystal symmetries to discuss the differences. Therefore, our results shed light on the existence of low-symmetry RP phases and make possible direct comparisons with future experiments.



Published in:
G. Zvejnieks, Y. Mastrikov, D. Gryaznov, Scientific Reports 13 (2023) 16446.
DOI: 10.1038/s41598-023-43381-7.

Paramagnetic radiation-induced radicals in calcium pyrophosphate polymorphs

A. Antuzevics[1,2], J. Cirulis[2], G. Krieke[2], D. Griesiute[1], A. Beganskiene[1], A. Kareiva[1], A. Dubauskas[3], V. Klimavicius[3], A. Zarkov[1]

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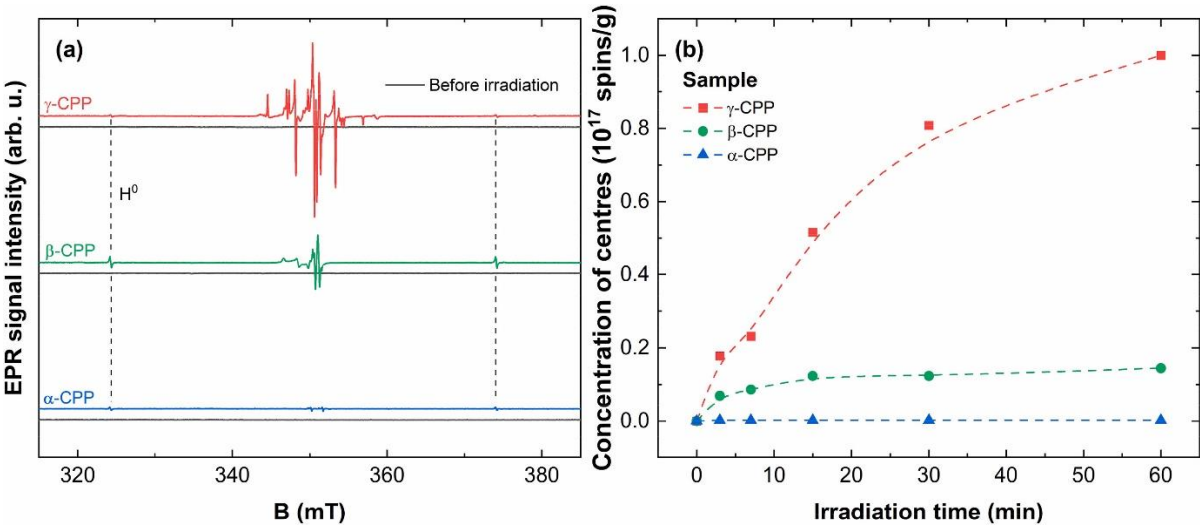
Calcium pyrophosphate ($Ca_2P_2O_7$) is a promising material for biomedical and optical applications; however, relatively little is documented on the radiation-induced point defects of the material. This study reports on the formation, identity, and properties of X-ray-induced radicals in γ-, β-, and α-polymorphs of $Ca_2P_2O_7$. Complementary thermally stimulated luminescence (TSL), electron paramagnetic resonance (EPR), and solid-state nuclear magnetic resonance (NMR) spectroscopy techniques were combined to reveal the effects of ionising radiation on each polymorph. The high-temperature polymorphs β-, and α- $Ca_2P_2O_7$ exhibited diminishing variety and intensity of EPR signals, whereas the opposite trend was observed in the TSL response. TSL glow curves consisted of multiple peaks in the temperature range of 20–350 ◦ C, with maximum emission intensity located at approximately 600 nm. Multiple electronic spin 1/2 paramagnetic centres were identified based on spin-Hamiltonian parameters determined from EPR spectra simulations. Annealing kinetics of the individual paramagnetic centres were determined to provide an interpretation of the complex nature of TSL glow curves. A decrease of the 31P spin-lattice relaxation T1 times after irradiation was detected for all $Ca_2P_2O_7$ polymorphs. The results highlight the importance of structure, morphology, and synthesis conditions on the formation of charge traps in $Ca_2P_2O_7$ and expand the knowledge base on the variety of radiation-induced radicals in phosphate materials.



Published in:
A.Antuzevics, J. Cirulis, G. Krieke, D. Griesiute, A. Beganskiene, A. Kareiva, A. Dubauskas, V. Klimavicius, A. Zarkov, Materials Chemistry and Physics 310 (2023) 128479.
DOI: 10.1016/j.matchemphys.2023.128479.

Peculiarities of the local structure in new medium- and high-entropy, low-symmetry tungstates

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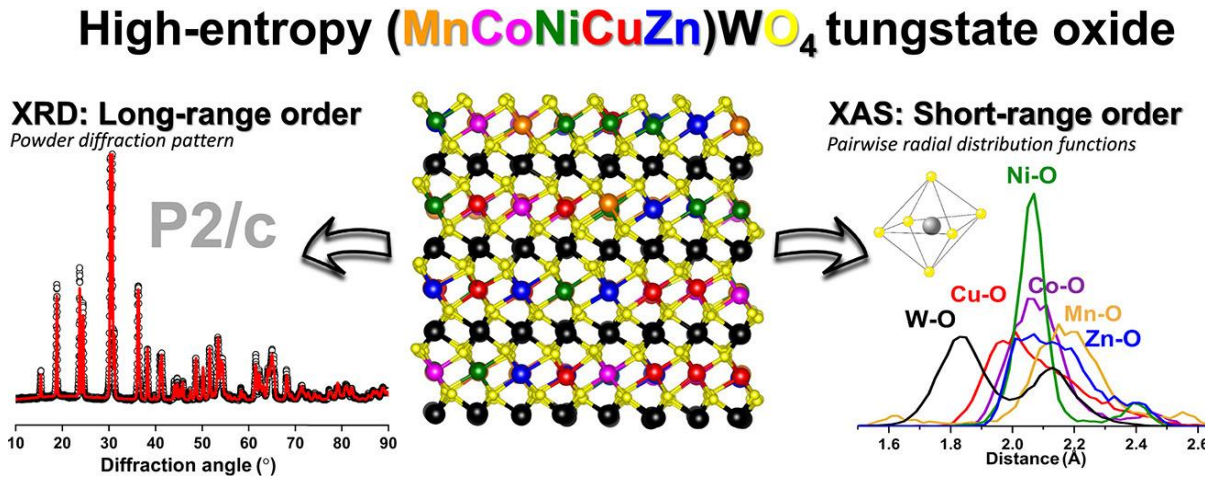
The concept of high-entropy materials (HEMs) – first proven for metallic systems – is now actively being transferred to other classes of non-metallic materials: carbides, nitrides, oxides, sulfides, etc. Although some HEMs are known to exhibit exceptional properties, numerous fundamental questions are yet to be clarified. The local chemical order is believed to play an important role in HEMs, although its influence on their macroscopic properties is not yet fully understood. So far, several attempts have been made to investigate HEMs using techniques sensitive to the local atomic structure, such as X-ray absorption spectroscopy.

New monoclinic (P2/c) tungstates – a medium-entropy tungstate, $(MnNiCuZn)WO_4$, and a high-entropy tungstate, $(MnCoNiCuZn)WO_4$ – were synthesized and characterized. Their phase purity and solid solution nature were confirmed by powder X-ray diffraction and Raman spectroscopy. X-ray absorption spectroscopy was used to probe the local structure around metal cations. The atomic structures based on the ideal solid solution model were optimized by a simultaneous analysis of the extended X-ray absorption fine structure spectra at multiple metal absorption edges – five for $(MnNiCuZn)WO_4$ and six for $(MnCoNiCuZn)WO_4$ – employing reverse Monte Carlo simulations. In both compounds, Ni^{2+} ions have the strongest tendency to organize their local environment and form slightly distorted $[NiO_6]$ octahedra, whereas Mn^{2+}, Co^{2+}, and Zn^{2+} ions have a strongly distorted octahedral coordination. The most intriguing result is that the shape of $[CuO_6]$ octahedra in $(MnNiCuZn)WO_4$ and $(MnCoNiCuZn)WO_4$ differs from that found in pure $CuWO_4$, where a strong Jahn–Teller distortion is present: $[CuO_6]$ octahedra become more regular with increasing degree of dilution.



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G. Bakradze, E. Welter, A. Kuzmin, Journal of Physics and Chemistry of Solids 172 (2023) 111052.
DOI: 10.1016/j.jpcs.2022.111052.

Vibrational spectra and lattice dynamics of the β-phase of white phosphorus

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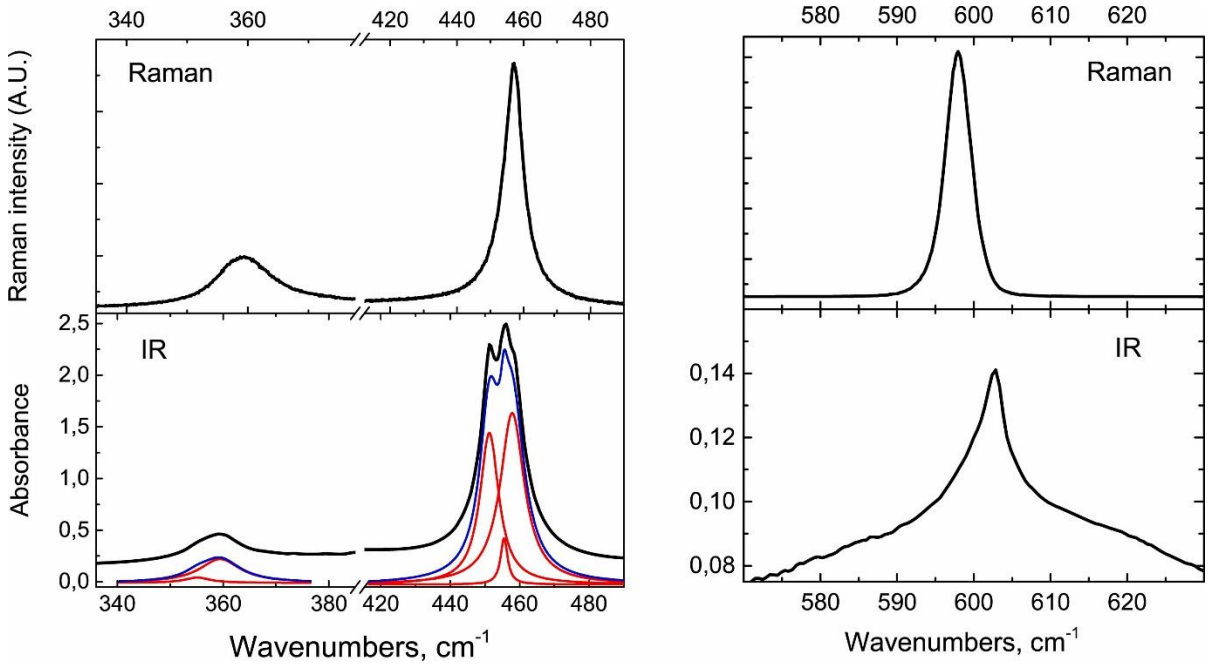
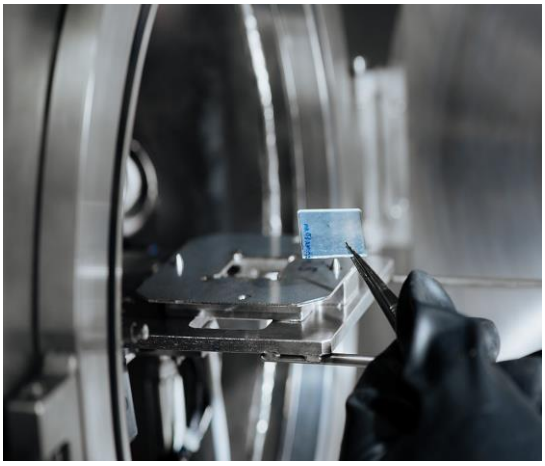
There are three known modifications of white phosphorus, which exist at different temperatures. The α-form exists at room temperature and is a plastic molecular crystal with the P_4 molecules dynamically rotating around their centers of gravity. A phase transition is known to occur at 196 K, at which the α-form transforms into the low-temperature β-form of white phosphorus. However, supercooling is possible, and the α→β transition can be delayed and occurs several degrees or even several tens of degrees below this temperature. This phase transition is reversible, and when the β-phase is heated, the β→α transition always occurs at a temperature of 196 K.

In this study, we report on a study of the α- and β-phases of white phosphorus using infrared and Raman spectroscopy. The spectra of the β-phase were measured at a temperature of 10 K with a sufficiently high resolution – allowing, for the first time, observation of the crystalline splitting of the bands corresponding to molecular vibrations. The band corresponding to the ν_1 (A1) vibration splits into six components. The bands corresponding to the ν_3 (F2) and the ν_2 (E) vibrations split into 17 and 12 components, respectively. The half-width (FWHM) of the bands in the infrared spectra range within 0.2–0.3 cm^{-1}, and the FWHM for the bands in Raman spectra is about 0.15 cm^{-1}. Based on ab initio calculations, symmetry analysis and our vibrational spectra, conclusions are drawn about the lattice dynamics of the β-phase of white phosphorus.



Published in:
G. Chikvaidze, J. Gabrusenoks, Journal of Physics and Chemistry of Solids 178 (2023) 111356.
DOI: 10.1016/j.jpcs.2023.111356.

II. Technology and experimental methods



Ultrafast laser writing in different types of silica glass

Yuhao Lei[1], Huijun Wang[1], Linards Skuja[2], Bodo Kühn[3], Bernhard Franz[3], Yuri Svirko[4], Peter G. Kazansky[1]

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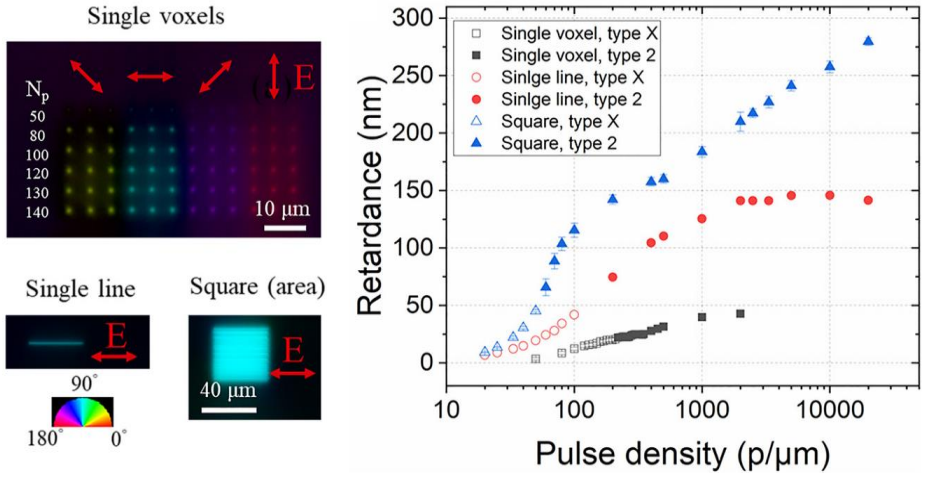
In the last few decades, the interaction of intense ultrashort light pulses with transparent materials has attracted considerable interest due to new phenomena associated with light-induced modification of materials and applications ranging from laser surgery, three-dimensional (3D) integrated optics, microfluidics, and optical data storage. In this study, it is demonstrated that ultrafast laser writing in silica glass depends on the grade of silica glass associated with the method of its manufacture. Moreover, laser-written modifications, in particular birefringent modifications, reveal a dependence on the geometry of writing, that is, the modification strength of voxels is smaller than that of single-line structures and multi-line scanned areas, which can be explained by free carrier diffusion and reduced electric field in scanning writing. The retardance of the scanned birefringent region produced in the regime of anisotropic nanopores formation in silica glass manufactured by vapor axial deposition (VAD) is about five times higher than that in an electrically fused sample at the same laser writing parameters, while the difference in retardance of a nanograting based modification in synthetic and fused silica is only about 10%. The phenomenon is interpreted in terms of the higher concentration of oxygen-deficient centers in the electrically fused silica glass, which can confine self-trapped holes and prevent nanopores formation. Improvement of high transmission optical elements is demonstrated in the VAD sample, and low-cost multiplexed optical data storage with higher capacity and readout accuracy is realized in the electrically fused silica glass.



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Y. Lei, H. Wang, L. Skuja, B. Kühn, B. Franz, Y. Svirko, P. G. Kazansky, Laser Photonics Rev 17 (2023) 2200978. DOI: 10.1002/lpor.202200978.

Two-step decoupled electrolysis approach based on pseudocapacitive WO_3 auxiliary electrode

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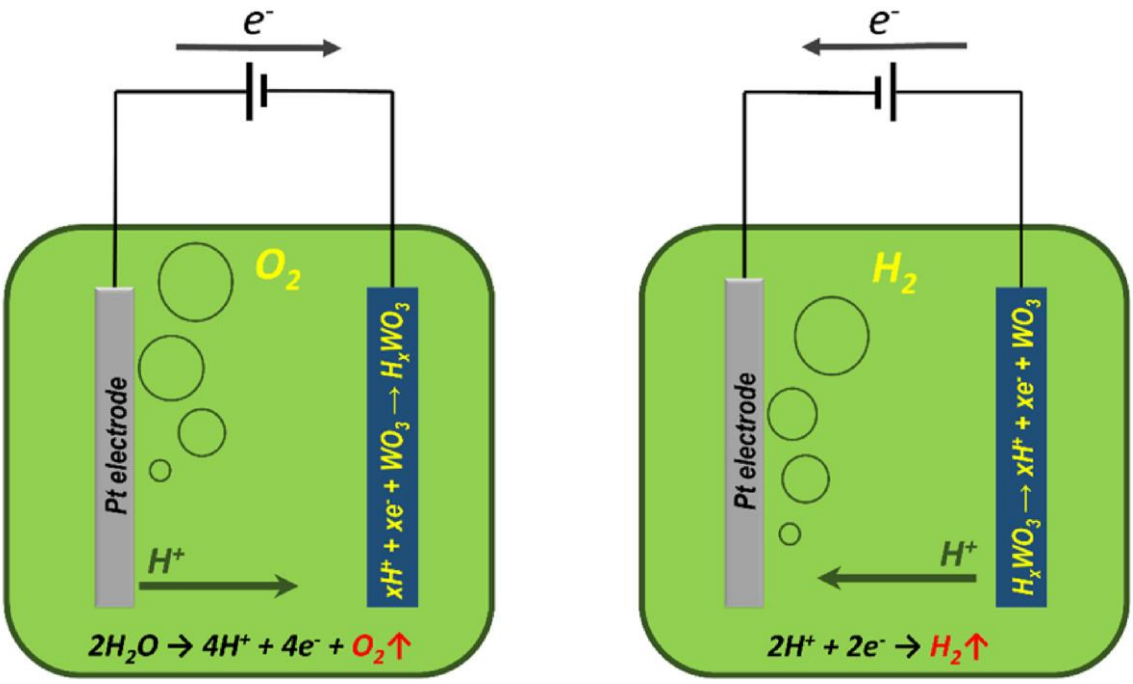
Hydrogen production via electrolysis is an efficient way to store excess energy from renewable energy plants, but electrolysis must be made more applicable. Conventional water electrolysis is complicated by a gas distribution and management system to prevent the mixing of H_2 and O_2 gases, which creates significant safety hazards. The use of membranes and diaphragms solves the gas mixing problem but reduces efficiency and directly affects the cost of hydrogen production. In this study, we show the decoupled water electrolysis concept, where hydrogen evolution and oxygen evolution are spatially and temporally separated using a WO_3 charge storage electrode as a red-ox mediator. Electrolysis is realized in two steps, where in the first step the oxygen evolution reaction (OER) and intercalation of H^+ in the WO_3 material take place. In the second step, the deintercalation of H+ from the WO_3 material and the reduction of H+ to H at the other electrode takes place. In the electrolysis process H_2 and O_2 gasses are produced with purity >99.9%. The overall efficiency of the electrolyzer is 65%.



Published in:
M. Vanags, M. Iesalnieks, L. Jēkabsons, A. Zukuls, A. Šutka, International Journal of Hydrogen Energy 48 (2023) 20551-20561. DOI: 10.1016/j.ijhydene.2023.03.035.

A stability study of transparent conducting $WO_3/Cu/WO_3$ coatings with antimicrobial properties

M. Zubkins[1], V. Vibornijs[1], E. Strods[1], I. Aulika[1], A. Zajakina[2], A. Sarakovskis[1], K. Kundzins[1], K. Korotkaja[2], Z. Rudevica[2], E. Letko[1], J. Purans[1]

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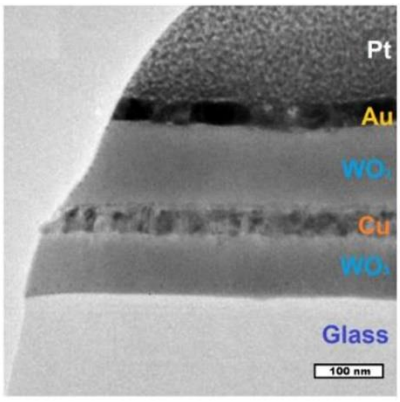
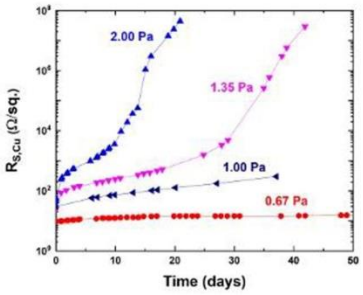
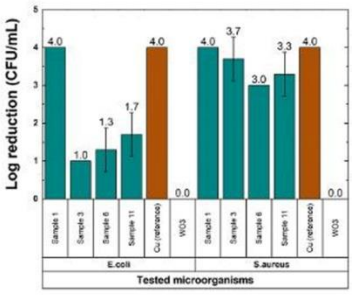
$WO_3/Cu/WO_3$ coatings are transparent electrodes, but their conductivity and transmittance have been observed to decrease with time. This paper reports the improved stability of $WO_3/Cu/WO_3$ coatings deposited by magnetron sputtering on glass and polyethylene terephthalate substrates. The stability issues due to Cu oxidation and migration can be addressed by adjusting the deposition parameters. Lowering the sputtering pressure results in denser WO_3 films, confirmed by spectroscopic ellipsometry, and thus more stable coatings. The coatings retain their properties in an inert atmosphere, indicating that Cu oxidation is the main reason for the decrease in conductivity, rather than its migration observed by X-ray photoelectron spectroscopy. Optical property modeling is used to optimize the thickness of the three-layer coatings to obtain the highest figure-of-merit for a transparent electrode. A structure of glass/WO_3 (70 nm)/Cu (10 nm)/WO_3 (45 nm) gives a sheet resistance of 14 Ω/sq. and a light transmittance of 65% at 600 nm. In addition, the antimicrobial properties of these coatings are revealed. A decrease of up to 10^5 of the gram-negative Escherichia coli and gram-positive Staphylococcus aureus bacterial colony formation units is found for several $WO_3/Cu/WO_3$-based coatings. In the case of the MS2 (Emesvirus zinderi) bacteriophage, a decrease in infectious particles for up to 10^4 plaque-forming units is obtained. The results indicate that more stable samples also had higher antimicrobial activity.



Cross section of $WO_3/Cu/WO_3$ coating



Evolution of sheet resistance of inner Cu film as a function of deposition pressure



Antibacterial tests

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M. Zubkins, V. Vibornijs, E. Strods, I. Aulika, A. Zajakina, A. Sarakovskis, K. Kundzins, K. Korotkaja, Z. Rudevica, E. Letko, J. Purans, Surfaces and Interfaces 41 (2023) 103259. DOI: 10.1016/j.surfin.2023.103259.

Extracellular Vesicles Isolation from Large Volume Samples Using a Polydimethylsiloxane-Free Microfluidic Device

C. Bajo-Santos[1], M. Priedols[1], P. Kaukis[1], G. Paidere[2], R. Gerulis-Bergmanis[1], G. Mozolevskis[2], A. Abols[1], R. Rimsa[2]

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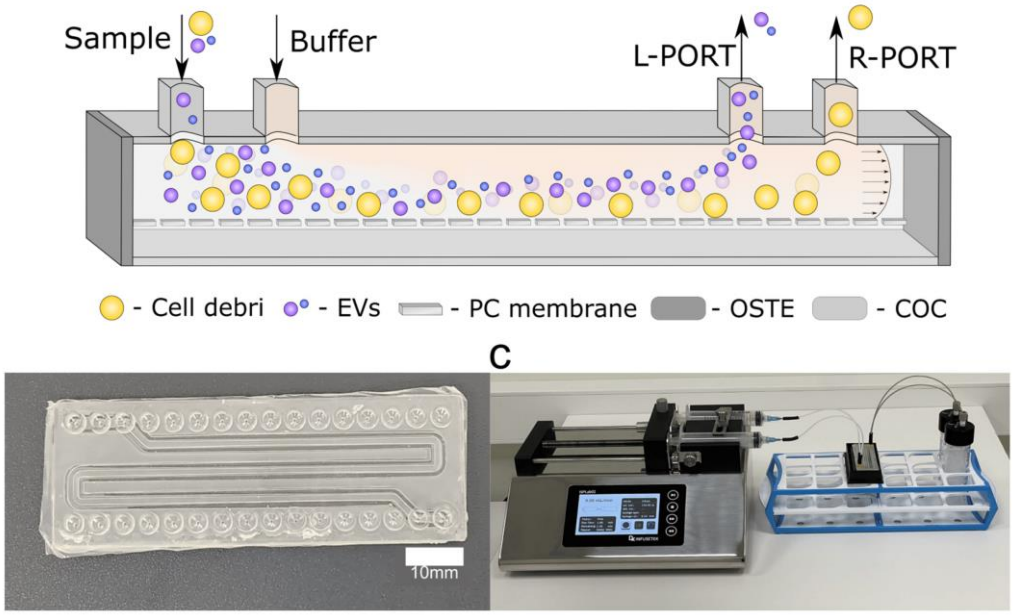
Extracellular vesicles (EV) have many attributes important for biomedicine; however, current EV isolation methods require long multi-step protocols that generally involve bulky equipment that cannot be easily translated to clinics. We aimed to design a new cyclic olefin copolymer–off-stoichiometry thiol-ene (COC–OSTE) asymmetric flow field fractionation microfluidic device that could isolate EV from high-volume samples in a simple and efficient manner. We tested the device with large volumes of urine and conditioned cell media samples, and compared it with the two most commonly used EV isolation methods. Our device was able to separate particles by size and buoyancy, and the attained size distribution was significantly smaller than other methods. This would allow for targeting EV size fractions of interest in the future. However, the results were sample-dependent, with some samples showing significant improvement over the current EV separation methods. We present a novel design for a COC–OSTE microfluidic device, based on bifurcating asymmetric flow field-flow fractionation (A4F) technology, which can isolate EV from large volume samples in a simple, continuous-flow manner. Its potential to be mass-manufactured increases the chances of implementing EV isolation in a clinical or industry-friendly setting, which requires high repeatability and throughput.



Published in:
C. Bajo-Santos, M. Priedols, P. Kaukis, G. Paidere, R. Gerulis-Bergmanis, G. Mozolevskis, A. Abols, R. Rimsa, International Journal of Molecular Sciences 24 (2023) 7971. DOI: 10.3390/ijms24097971.

Reactive pulsed direct current magnetron sputtering deposition of semiconducting yttrium oxide thin film in ultralow oxygen atmosphere

H. Arslan[1], I. Aulika[1], A. Sarakovskis[1], L. Bikse[1], M. Zubkins[1], A. Azarov[2], J. Gabrusenoks[1], J. Purans[1]

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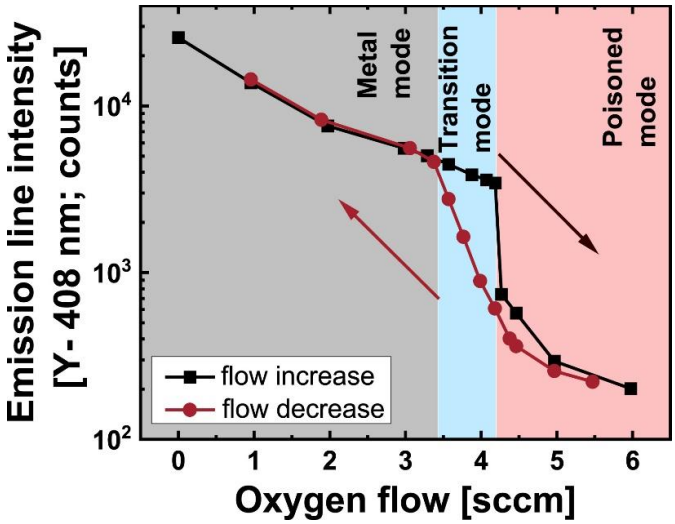
Because of their unusual valence band electronic configuration ($4f^{n-1}\,5d^{0,1}\,6s^2$; n = 1-15), rare earth elements have become, over the last decades, one of the major interesting research subjects in science and crucial components in high-tech industry/products such as catalysis field (e.g. Ce), hybrid engines (e.g. Dy), neutron detection (e.g. Sm, Eu), and fusion reactors/nuclear plants (e.g. Y). An experimental investigation was conducted to explore spectroscopic and structural characterization of semiconducting yttrium oxide thin film deposited at 623 K (±5K) utilizing reactive pulsed direct current magnetron sputtering. Based on the results obtained from both x-ray diffraction and transmission electron microscope measurements, yttrium monoxide is very likely formed in the transition region between β-Y_2O_3 and α- Y_2O_3, and accompanied by the crystalline Y_2O_3. Resulting of either the low energy separation between 4d and 5s orbitals and/or different spin states of the corresponding orbitals' sublevels, the stability of monoxide is most presumably self-limited by the size of the crystal in thermodynamic terms. This behavior develops a distortion in the structure of the crystal compared to the metal oxide cubic structure and it also effectuates the arrangement in the nanocrystalline/amorphous phase. In addition to this, spectroscopic ellipsometry denotes that the semiconducting yttrium oxide has the dominant, mostly amorphous, formation character over crystalline Y_2O_3. Our purpose, by means of the current findings, is to advance the understanding of formation kinetics/conditions of yttrium with an unusual valency (2+).



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H. Arslan, I. Aulika, A. Sarakovskis, L. Bikse, M. Zubkins, A. Azarov, J. Gabrusenoks, J. Purans, Vacuum 211 (2023) 111942. DOI: 10.1016/j.vacuum.2023.111942.

Deposition of Ga_2O_3 thin films by liquid metal target sputtering

M. Zubkins[1], V. Vibornijs[1], E. Strods[1], E. Butanovs[1], L. Bikse[1], M. Ottosson[2], A. Hallen[3], J. Gabrusenoks[1], J. Purans[1], A. Azens[4]

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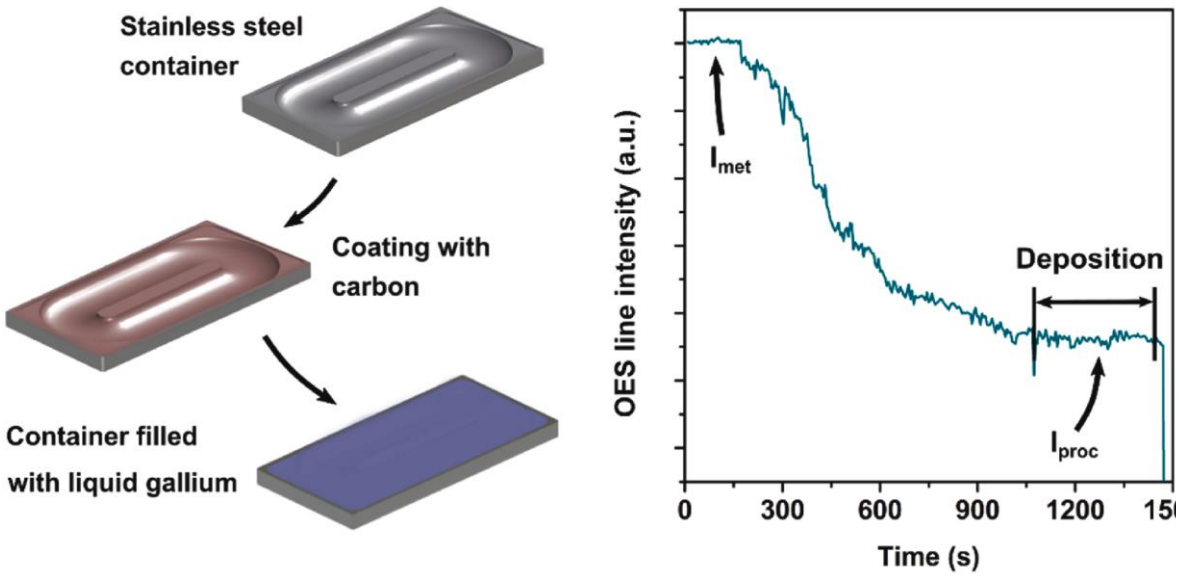
Gallium oxide (Ga_2O_3) has attracted a lot of attention as an ultra-wide bandgap semiconductor. This study reports on the deposition of amorphous and crystalline thin films of Ga_2O_3 by reactive pulsed direct current magnetron sputtering from a liquid gallium target onto fused (f-) quartz and c plane (c-) sapphire substrates, where the temperature of the substrate is varied from room temperature (RT) to 800 °C. The deposition rate (up to 37 nm/min at RT on f-quartz and 5 nm/min at 800 °C on c-sapphire) is two to five times higher than the data given in the literature for radio frequency sputtering. Deposited onto unheated substrates, the films are X-ray amorphous. Well-defined X-ray diffraction peaks of β-Ga_2O_3 start to appear at a substrate temperature of 500 °C. Films grown on c-sapphire at temperatures above 600 °C are epitaxial. However, the high rocking curve full width at half maximum values of ≈2.4–2.5° is indicative of the presence of defects. A dense and void-free microstructure is observed in electron microscopy images. Composition analysis shows stoichiometry close to Ga_2O_3 and no traces of impurities. The optical properties of low absorptance (<1%) in the visible range and an optical band gap of approximately 5 eV are consistent with the data in the literature for Ga_2O_3 films produced by other deposition methods.



Published in:
M. Zubkins, V. Vibornijs, E. Strods, E. Butanovs, L. Bikse, M. Ottosson, A. Hallen, J. Gabrusenoks, J. Purans, A. Azens, Vacuum 209 (2023) 111789. DOI: 10.1016/j.vacuum.2022.111789.

Hydrothermal Synthesis and Properties of Yb^{3+}/Tm^{3+} Doped Sr_2LaF_7 Upconversion Nanoparticles

B. Milicevic[1], J. Periša[1], Z. Ristic[1], K. Milenkovic[1], Ž. Antic[1], K. Smits[2], M. Kemere[2], K. Vitols[2], A. Sarakovskis[2], M.D. Dramicanin[1]

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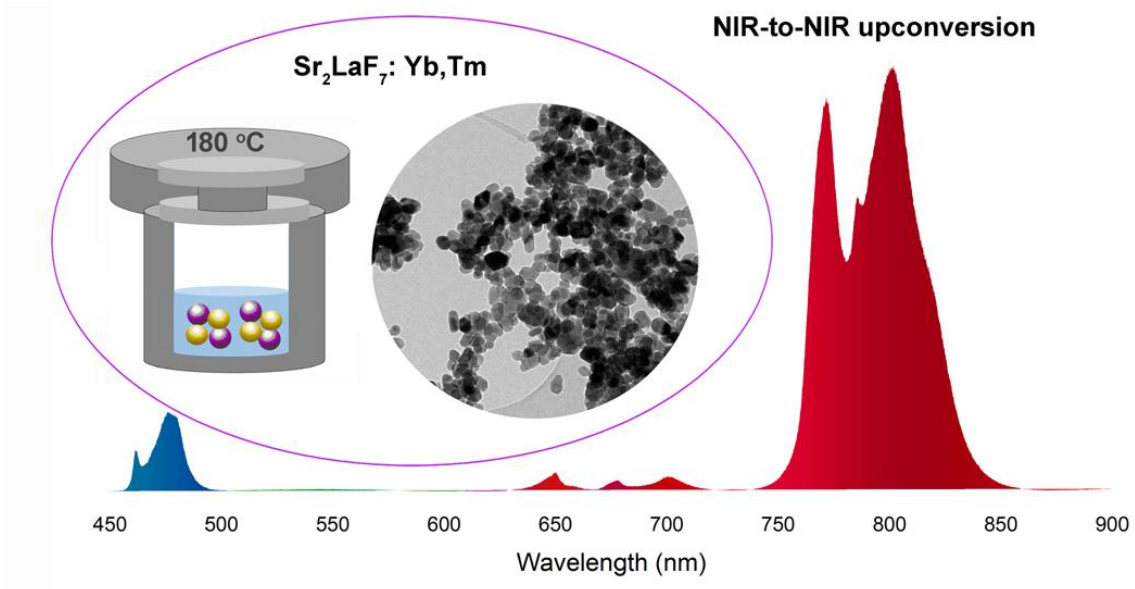
Upconversion (UC) phosphor materials doped or co-doped with trivalent lanthanide (Ln^{3+}) ions have drawn considerable attention, since four-electron configurations of Ln^{3+} ions should split by electron-electron repulsion and spin-orbit coupling, resulting in a rich energy-level pattern that can be easily populated by the near-infrared (NIR) laser source. In this study, we report the procedure for hydrothermal synthesis of ultrasmall Yb^{3+}/Tm^{3+} co-doped Sr_2LaF_7 (SLF) upconversion phosphors. These phosphors were synthesized by varying the concentrations of Yb^{3+} (x = 10, 15, 20, and 25 mol%) and Tm^{3+} (y = 0.75, 1, 2, and 3 mol%) with the aim to analyze their emissions in the near IR spectral range. According to the detailed structural analysis, Yb3+ and Tm^{3+} occupy the La^{3+} sites in the SLF host. The addition of Yb^{3+}/Tm^{3+} ions has a huge impact on the lattice constant, particle size, and PL emission properties of the synthesized SLF nanophosphor. The results show that the optimal dopant concentrations for upconversion luminescence of Yb^{3+}/Tm^{3+} co-doped SLF are 20 mol% Yb^{3+} and 1 mol% Tm^{3+} with EDTA as the chelating agent. Under 980 nm light excitation, a strong upconversion emission of Tm3+ ions around 800 nm was achieved. In addition, the experimental photoluminescence lifetime of Tm^{3+} emission in the SLF host is reported. This study discovered that efficient near IR emission from ultrasmall Yb^{3+}/Tm^{3+} co-doped SLF phosphors may have potential applications in the fields of fluorescent labels in bioimaging and security applications.



Published in:
B. Milicevic, J. Periša, Z. Ristic, K. Milenkovic, Ž. Antic, K. Smits, M. Kemere, K. Vitols, A. Sarakovskis, M.D. Dramicanin, Nanomaterials 13 (2023) 30. DOI: 10.3390/nano13010030.

Effect of Post-Printing Cooling Conditions on the Properties of ULTEM Printed Parts

T. Glaskova-Kuzmina[1,2], D. Dejus[1], J. Jatnieks[1], A. Aniskevich[2], J. Sevcenko[2], A. Sarakovskis[3], A. Zolotarjovs[3]

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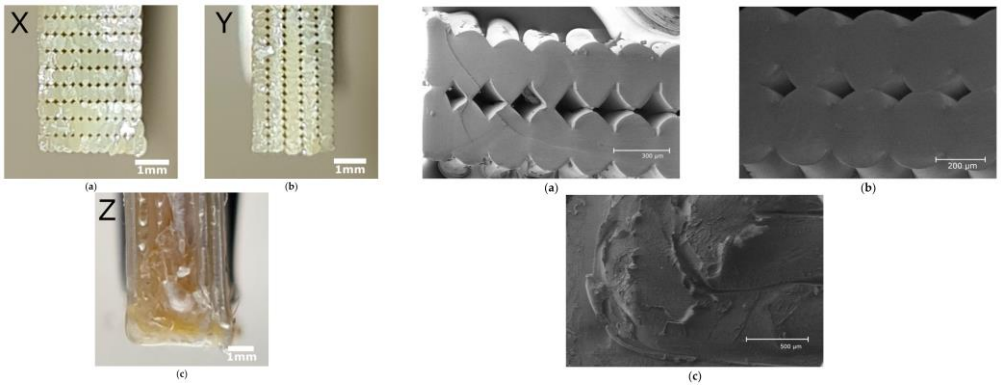
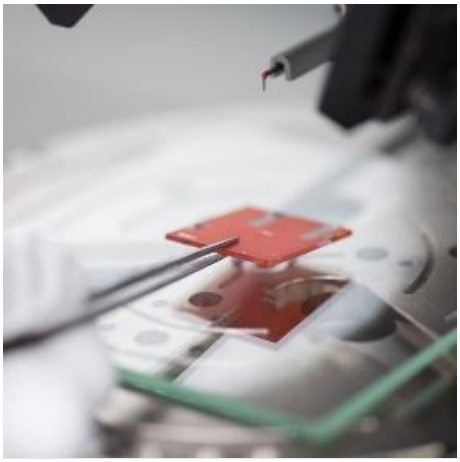
Additive manufacturing (AM) of both single- and multi-material structures has recently been applied to efficiently produce complex structures, thus saving production time and resources. AM offers unprecedented levels of freedom for the design and application of 3D-printed polymer materials, e.g., in automotive, aerospace, biomedical, and dentistry fields. Currently, fused deposition modeling (FDM) is one of the AM technologies that has been extensively applied in the manufacture of 3D-printed polymer parts. During this process, a polymer is extruded through a heated nozzle and deposited in a semi-molten state to create the required shape via sequential build-up of layered depositions.

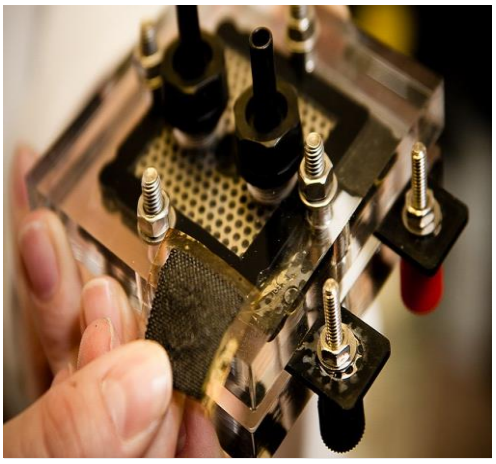
This study aimed to estimate the effect of post-printing cooling conditions on the tensile and thermophysical properties of ULTEM® 9085 printed parts processed by fused deposition modeling (FDM). Three different cooling conditions were applied after printing Ultem samples: from 180 ◦C to room temperature (RT) for 4 h in the printer (P), rapid removal from the printer and cooling from 200 ◦C to RT for 4 h in the oven (O), and cooling at RT (R). Tensile tests and dynamic mechanical thermal analysis (DMTA) were carried out on samples printed in three orthogonal planes to investigate the effect of the post-printing cooling conditions on their mechanical and thermophysical properties. Optical microscopy was employed to relate the corresponding macrostructure to the mechanical performance of the material. The results obtained showed almost no difference between samples cooled either in the printer or oven and a notable difference for samples cooled at room temperature. Moreover, the lowest mechanical performance and sensitivity to the thermal cooling conditions were defined for the Z printing direction due to the anisotropic nature of FDM and debonding among layers.



Published in:
T. Glaskova-Kuzmina, D. Dejus, J. Jatnieks, A. Aniskevich, J. Sevcenko, A. Sarakovskis, A. Zolotarjovs, Polymers 15 (2023) 324. DOI: 10.3390/polym15020324.

III. Applications: applied research of materials for sensors, scintillators, detectors, materials for photonics and electronics, and materials for energy harvesting and storage





Photocatalytic water splitting of improved strontium titanate for simultaneous separation of H_2 in a twin photoreactor

Yu-Yang Tai[1], Jeffrey C.S. Wu[1], Wen-Yueh Yu[1], Marjeta Maček Kržmanc[2], Eugene Kotomin[3]

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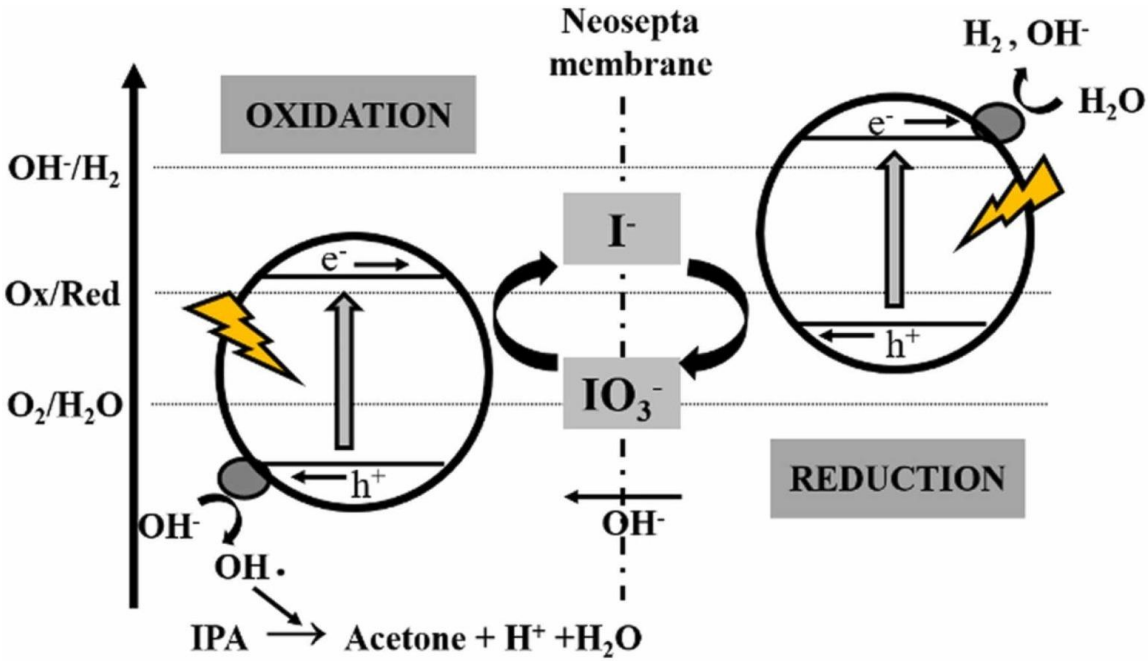
Nowadays, due to the burning of fossil fuels, global warming and the rising sea level have threatened the creatures on the earth. Many efforts have been made to develop renewable energies like solar, bioenergy, and wind energy to deal with the dilemma. Among all, photocatalysis has been considered a promising technology for utilizing solar energy.

In this study, a core-shell structural Rh-CrO_x loaded on Al^{3+} doped strontium titanate ($SrTiO_3$) was used for photocatalytic water splitting. A specially designed twin photoreactor, which integrates the water splitting and the degradation of isopropanol, can simultaneously carry out the degradation of isopropanol and hydrogen production. A flux method was conducted to prepare Rh@CrO_3 cocatalyst on Al^{3+} doped high-crystallinity strontium titanate for the photocatalyst of hydrogen evolution. Nearly 1200 µmole/g of hydrogen was evolved in photocatalytic whole water splitting in five hours under simulated AM 1.5 G sunlight. Pt-loaded WO_3 was utilized to degrade 100 ppm isopropanol solution. The above photocatalysts were used in the twin reactor with electron-mediator I^-/IO^{3-} and a Neosepta anion-exchanged membrane. Hydrogen evolution of 1102 µmole/g and isopropanol removal of 10.1% were achieved in five hours, indicating the rate-limiting H_2 rate was overcome. The quantum efficiencies on the hydrogen-evolution and degradation sides were estimated to be 0.102% and 0.123%, respectively.



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Y.-Y. Tai, J. C.S. Wu, W.-Y. Yu, M. M. Kržmanc, E. Kotomin, Applied Catalysis B: Environmental 324 (2023) 122183. DOI: 10.1016/j.apcatb.2022.122183.

Electrochemical properties of bismuth chalcogenide/MXene/CNT heterostructures for application in Na-ion batteries

R. Meija[1], V. Lazarenko[1,2], Y. Rublova[1], A. Kons[1], V. Voikiva[1], J. Andzane[1], O. Gogotsi[3], I. Baginskiy[3], V. Zahorodna[3], A. Sarakovskis[4], A. Pludons[5], A. Sutka[5], A. Viksna[6], D. Erts[1,6]

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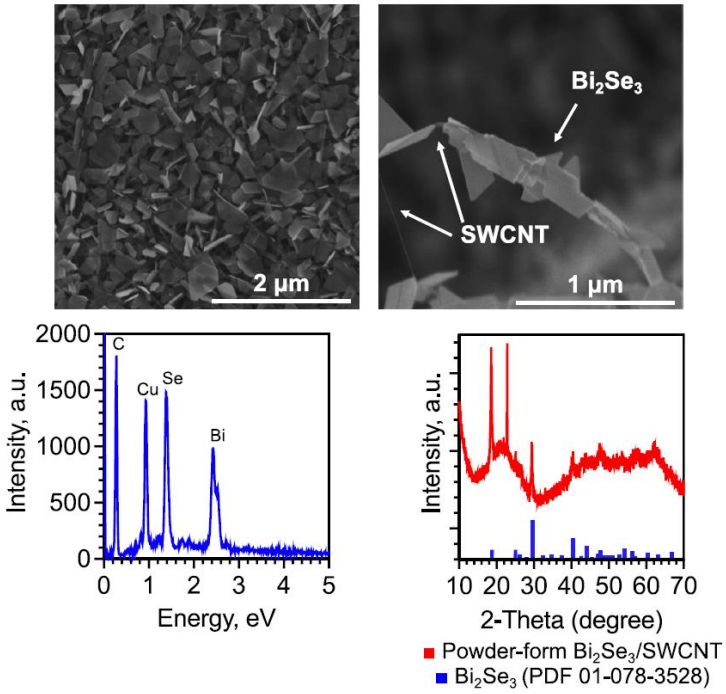
The development of high-performance anodes for sodium-ion batteries (SIBs) has recently attracted great attention. Most of the proposed anode materials for SIB systems suffer from insufficient electrical and mechanical contact of the active material with the current collector causing low reversible capacity and short lifespan. To solve this issue, an innovative approach could be the direct synthesis of the active material around and on the top of an electrically conductive network. The nanostructuring with SWCNTs and MXenes increases the active surface area, improves expansion/contraction properties, and establishes direct mechanical and electrical contact. In this work, the performance of binder-free Bi_2Se_3/SWCNT and Bi_2Se_3/MXene/SWCNT anode materials, which were synthesized by the direct physical vapor deposition of Bi_2Se_3 nanostructures on SWCNT and MXene/SWCNT network systems, was investigated. The results showed that the Bi_2Se_3/SWCNT electrode with the mass ratio of (1:1) exhibits excellent rate performance and high discharge capacity in the short-term (0.1 A g^{-1}) and long-term (5.0 A g^{-1}) cycling by delivering 247 and 120 mAh g^{-1} respectively demonstrating its perspectives for the application as an anode in SIBs



Published in:
R. Meija, V. Lazarenko, Y. Rublova, A. Kons, V. Voikiva, J. Andzane, O. Gogotsi, I. Baginskiy, V. Zahorodna, A. Sarakovskis, A. Pludons, A. Sutka, A. Viksna, D. Erts, Sustainable Materials and Technologies 38 (2023) e00768. DOI: 10.1016/j.susmat.2023.e00768.

Sb_2S_3 Thin-Film Solar Cells Fabricated from an Antimony Ethyl Xanthate Based Precursor in Air

J.S. Eensalu[1,2], S. Mandati[3], C.H. Don[4], H. Finch[4], V.R. Dhanak[4], J.D. Major[4], R. Grzibovskis[5], A. Tamm[5], P. Ritslaid[5], R. Josepson[6], T. Käämbre[2,7], A. Vembris[5], N. Spalatu[8], M. Krunks[8], I. Oja Acik[8]

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Sb_2S_3 has been a potential candidate for solar PVs and the efficiency of planar Sb_2S_3 thin-film solar cells has witnessed a reasonable rise from 5.77% in 2014 to 8% in 2022. Herein, the aim is to bring new insight into Sb_2S_3 solar cell research by investigating how the bulk and surface properties of the Sb_2S_3 absorber and the current–voltage and deep-level defect characteristics of solar cells based on these films are affected by the ultrasonic spray pyrolysis deposition temperature and the molar ratio of thiourea to SbEX in solution. The properties of the Sb_2S_3 absorber are characterized by bulk- and surface-sensitive methods. Solar cells are characterized by temperature-dependent current–voltage, external quantum efficiency, and deep-level transient spectroscopy measurements. In this paper, the first thin-film solar cells based on a planar Sb_2S_3 absorber grown from antimony ethyl xanthate (SbEX) by ultrasonic spray pyrolysis in air are demonstrated. Devices based on the Sb_2S_3 absorber grown at 200 °C, especially from a solution of thiourea and SbEX in a molar ratio of 4.5, perform the best by virtue of suppressed surface oxidation of Sb_2S_3, favorable band alignment, Sb-vacancy concentration, a continuous film morphology, and a suitable film thickness of 75 nm, achieving up to 4.1% power conversion efficiency, which is the best efficiency to date for planar Sb_2S_3 solar cells grown from xanthate-based precursors. Our findings highlight the importance of developing synthesis conditions to achieve the best solar cell device performance for an Sb_2S_3 absorber layer pertaining to the chosen deposition method, experimental setup, and precursors.

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J.S. Eensalu, S. Mandati, C.H. Don, H. Finch, V.R. Dhanak, J.D. Major, R. Grzibovskis, A. Tamm, P. Ritslaid, R. Josepson, T. Käämbre, A. Vembris, N. Spalatu, M. Krunks, I. Oja Acik, ACS Appl. Mater. Interfaces 15 (2023) 42622–42636. DOI: 10.1021/acsami.3c08547.

Tribovoltaic Performance of TiO_2 Thin Films: Crystallinity, Contact Metal, and Thermoelectric Effects

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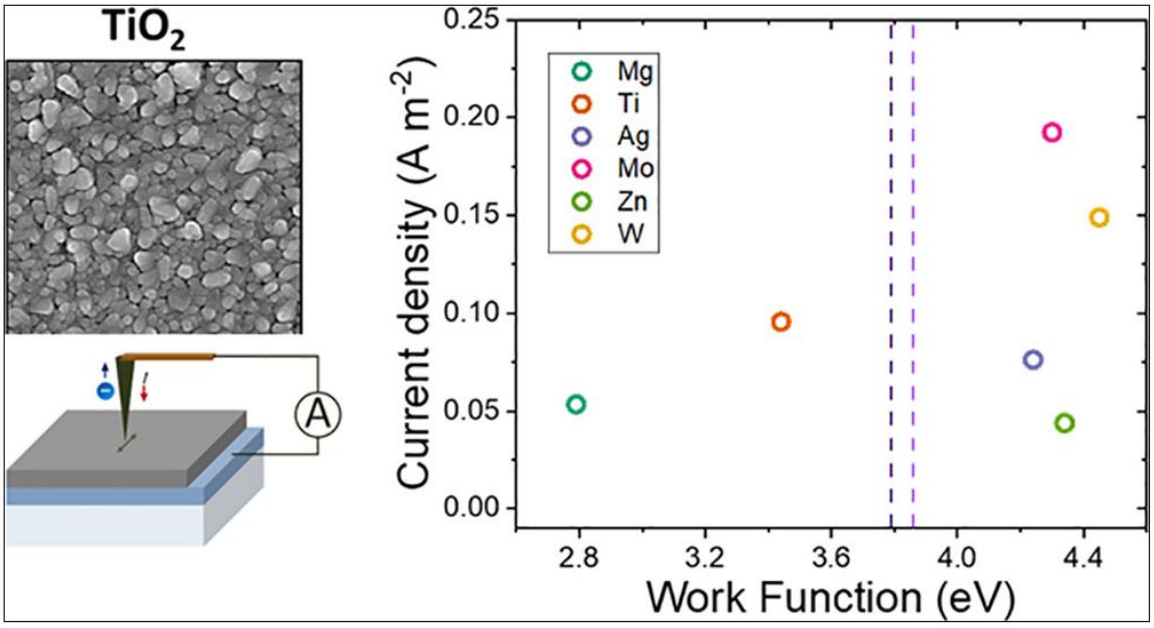
Tribovoltaic devices are attracting increasing attention as motion-based energy harvesters due to the high local current densities that can be generated. However, while these tribovoltaic devices are being developed, debate remains surrounding their fundamental mechanism. Here, we fabricate thin films from one of the world's most common oxides, TiO_2, and compare the tribovoltaic performance under contact with metals of varying work functions, contact areas, and applied pressure. The resultant current density shows little correlation with the work function of the contact metal and a strong correlation with the contact area. Considering other effects at the metal–semiconductor interface, the thermoelectric coefficients of different metals were calculated, which showed a clear correlation with the tribovoltaic current density. On the microscale, molybdenum showed the highest current density of 192 mA cm^{-2}. This work shows the need to consider a variety of mechanisms to understand the tribovoltaic effect and design future exemplar tribovoltaic devices.



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A review of the degradation mechanisms of NCM cathodes and corresponding mitigation strategies

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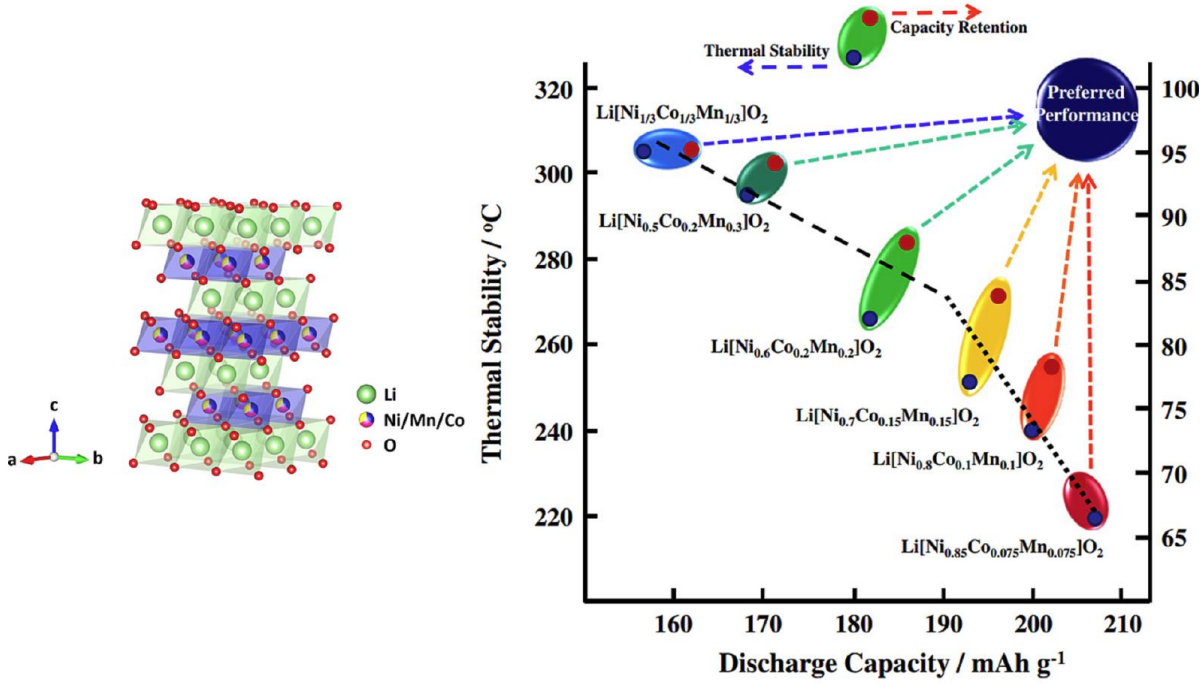
Li-ion batteries (LIBs) are the most widely used form of energy storage in mobile electronic devices and electric vehicles. Li-ion battery cathodes with the composition $LiNi_xMn_yCo_zO_2$ (NCMs) currently display some of the most promising electrochemical characteristics for high-performance LIBs. NCM compositions with high nickel content (x > 0.8) exhibit the largest specific capacity while undergoing fast degradation and presenting safety issues. As the main degradation mechanisms of NCM materials and the mitigation of their degradation, are still subjects of many ongoing studies, this work summarizes the current knowledge on the subject. Here, the existing literature is reviewed to present the structural and electrochemical degradation of NCM with varying Ni stoichiometries (NCM111, NCM622, NCM811, and beyond). Routes for hindering the degradation of NCM are discussed as a function of Ni content in NCM and include doping, application of protective coatings, and engineering of the microstructure. A comprehensive understanding of the main degradation pathways of NCM is key to applying the most appropriate mitigation strategies and advancing towards higher energy NCM materials with longer cycle-life.



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Filterless Visible-Range Color Sensing and Wavelength-Selective Photodetection Based on Barium/Nickel Codoped Bandgap-Engineered Potassium Sodium Niobate Ferroelectric Ceramics

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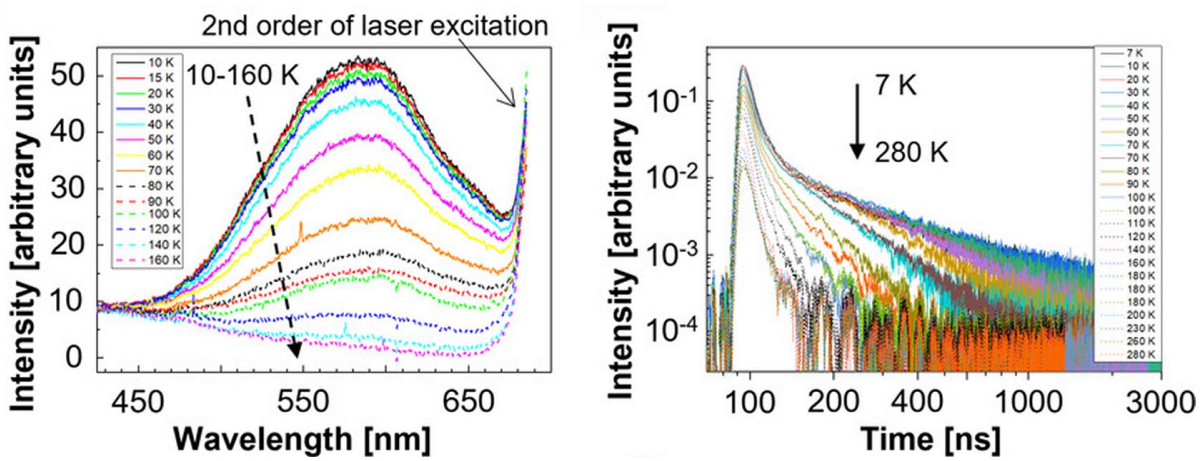
Photosensors, photodetectors, or color sensors are key components for various optical and optoelectronic applications. Semiconductor-based photodetection has been a dominator which is excellent at measuring the photon intensity of incident light. However, the wavelength of the incident light to be measured must be known beforehand and it mostly depends on auxiliary methods to filter unknown wavelengths. Herein, an alternative but simple mechanism that uses a monolithic, bandgap-engineered photoferroelectric ceramic to blindly determine the wavelength and intensity of incident light at the same time is demonstrated. The photoferroelectric compound is Ba- and Ni-codoped (K,Na)NbO_3 exhibiting a direct bandgap of ≈2 eV and a spontaneous polarization of ≈0.25 C m^{-2}. The band–band charge carrier transition is confirmed by multiple characterization methods of photoluminescence, photodielectric spectroscopy, and photoconductivity. The existent optoelectrical cumulative effect enabled by the simultaneous narrow bandgap and strong ferroelectricity allows to reliably distinguish the wavelengths of 405, 552, and 660 nm as well as the power density ranging from ≈0.1 to 10 W cm^{-2}, with the photoresponsivity of up to 60 µA W^{-1}. Consequently, this work proposes an alternative to semiconductor-based counterparts for filterless, wavelength-selective photodetection and color sensing.



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Development of Bi_2S_3 thin film solar cells by close-spaced sublimation and analysis of absorber bulk defects via in-depth photoluminescence analysis

M. Koltsov[1], S.V. Gopi[1], T. Raadik[1], J. Krustok[1], R. Josepson[2], R. Gržibovskis[3], A. Vembris[3], N. Spalatu[1]

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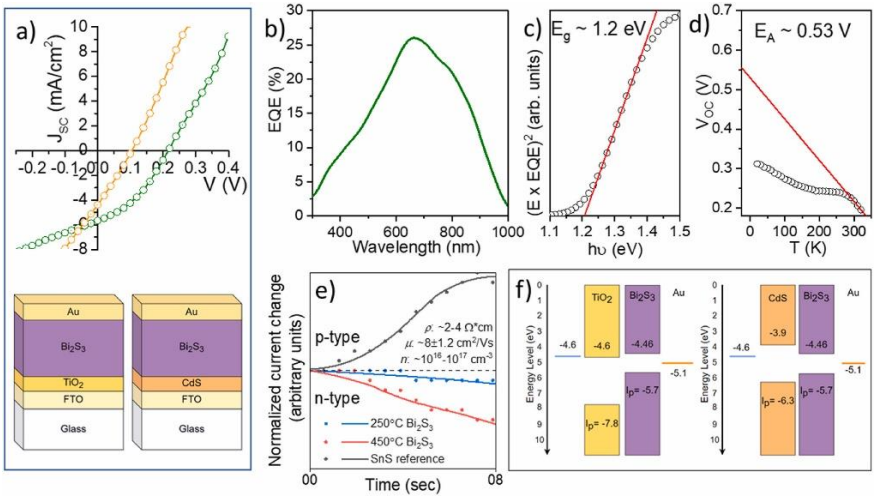
The emergence of new PV applications in society requires the design of new materials and devices based on green and earth-abundant elements, with a different set of properties and wider applicability. In this perspective, Bi_2S_3 semiconductor material have gained attention as a defect-tolerant, non-toxic, and highly stable material for earth-abundant thin film PV technologies. Related to Bi_2S_3 non-toxic nature, so far it has been very popular to synthesize the material by chemical solution routes, while little research efforts have been dedicated to absorber deposition by physical deposition techniques. In particular, there are no studies on absorber development via rapid, high-volume, and in-line close-spaced sublimation technique. Moreover, in-depth analysis of material defects employing low temperature-dependent photoluminescence (PL) remains largely unexplored. In this work, we systematically study the impact of close-spaced sublimation (CSS) conditions on Bi_2S_3 absorber growth on various substrates, employing a wide range of source (400–600 °C) and substrate (200–400 °C) temperatures. CSS source temperature of 550 °C and substrate temperature of 400–450 °C were identified as optimal temperatures (grown either on glass, TiO_2, or CdS substrates), allowing the fabrication of uniform and dense Bi_2S_3 films with enhanced [221]-oriented grains. For the first time, a proof of concept solar cell with CSS Bi_2S_3 is demonstrated and an in-depth analysis of the interrelation between grain structure, interface recombination, and device performance is provided. Employing low-temperature dependence PL, new and complementary insights on possible defects and recombination mechanisms are presented.



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Low processing temperatures explored in Sb_2S_3 solar cells by close-spaced sublimation and analysis of bulk and interface related defects

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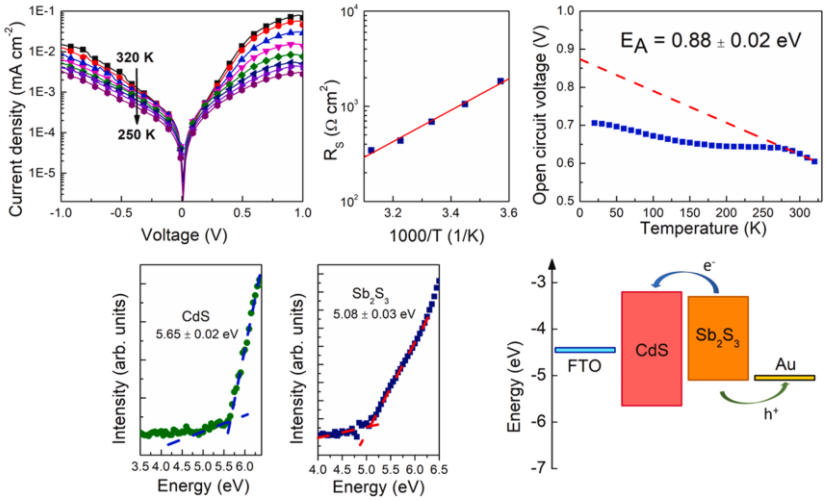
Antimony trisulfide (Sb_2S_3) is a promising photovoltaic absorber, which has so far been fabricated mainly by chemical deposition methods. Despite its aptness for congruent sublimation, fewer research efforts have been made on low-temperature Sb_2S_3 processing by physical methods. In this regard, recent studies show a large variation in the processing temperature of Sb_2S_3 films, which overall brings into question the need for higher substrate temperatures (>350 °C). Furthermore, an in-depth analysis of the defect structure of Sb_2S_3 employing temperature-dependent admittance spectroscopy (TAS) and photoluminescence (PL) remains largely unexplored. In this work, we systematically study the effect of close-spaced sublimation (CSS) substrate temperature on Sb_2S_3 absorber growth, employing a wide temperature range of 240–400 °C. Temperatures above 320 °C caused cracking phenomena in the Sb_2S_3 absorber film, proving the inappropriateness of higher processing temperatures. CSS processing temperature of 300 °C was found optimal, producing crack-free Sb_2S_3 films with the increased presence of (hk1) planes, and achieving the best CdS/ Sb_2S_3 device with photoconversion efficiency of 3.8%. TAS study revealed two deep defects with activation energies of 0.32 eV and 0.37 eV. Low-temperature PL measurement revealed a band-to-band emission at 1.72 eV and a broad band peaked at 1.40 eV, which was assigned to a donor-acceptor pair recombination. Temperature-dependent I-V analysis showed that recombination at the CdS– Sb_2S_3 interface remains a large limitation for the device efficiency.



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4.9% Efficient Sb_2S_3 Solar Cells from Semitransparent Absorbers with Fluorene-Based Thiophene-Terminated Hole Conductors

S. Mandati[1], N. Juneja[1], A. Katerski[1], A. Jegorovė[2], R. Grzibovskis[3], A. Vembris[3], T. Dedova[1], N. Spalatu[1], A. Magomedov[2], S. Karazhanov[4], V. Getautis[2], M. Krunks[1], I. Oja Acik[1]

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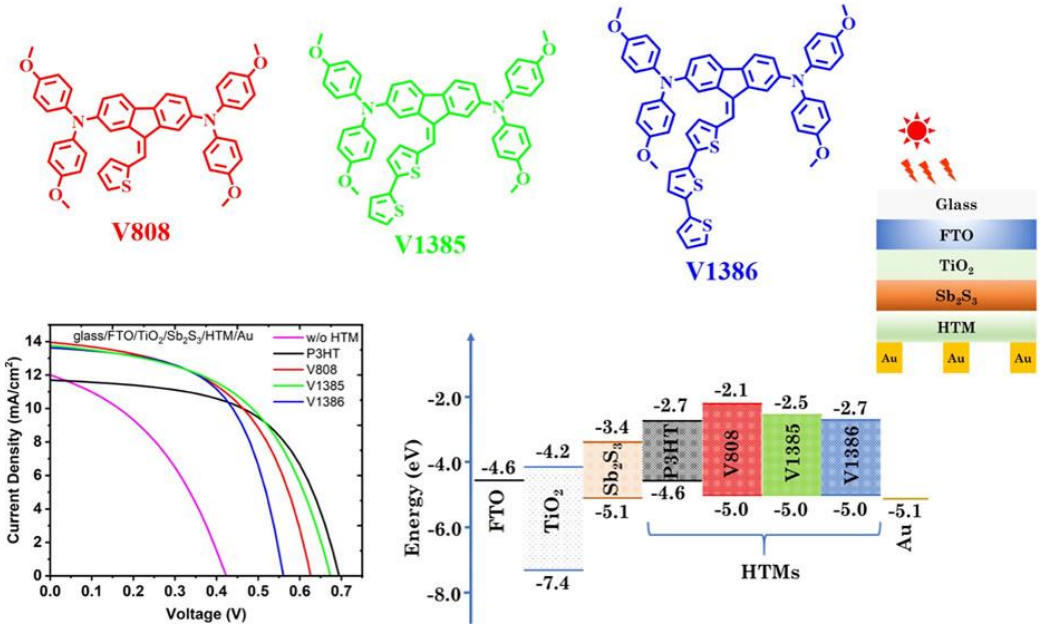
Fluorene-based hole transport materials (HTMs) with terminating thiophene units are explored, for the first time, for antimony sulfide (Sb_2S_3) solar cells. These HTMs possess largely simplified synthesis processes and high yields compared to the conventional expensive hole conductors making them reasonably economical. The thiophene unit-linked HTMs have been successfully demonstrated in ultrasonic spray-deposited Sb_2S_3 solar cells resulting in efficiencies in the range of 4.7–4.9% with an average visible transmittance (AVT) of 30–33% (400–800 nm) for the cell stack without metal contact, while the cells fabricated using conventional P3HT have yielded an efficiency of 4.7% with an AVT of 26%. The study puts forward cost-effective and transparent HTMs that avoid a post-coating activation at elevated temperatures like P3HT, devoid of parasitic absorption losses in the visible region and are demonstrated to be well aligned for the band edges of Sb_2S_3 thereby ascertaining their suitability for Sb_2S_3 solar cells and are potential candidates for semitransparent applications.



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S. Mandati, N. Juneja, A. Katerski, A. Jegorovė, R. Grzibovskis, A. Vembris, T. Dedova, N. Spalatu, A. Magomedov, S. Karazhanov, V. Getautis, M. Krunks, I. Oja Acik, ACS Appl. Energy Mater. 6 (2023) 3822–3833. DOI: 10.1021/acsaem.2c04097.

Structure and persistent luminescence of novel Pr-doped $Mg_3Lu_2Ge_3O_{12}$ garnet

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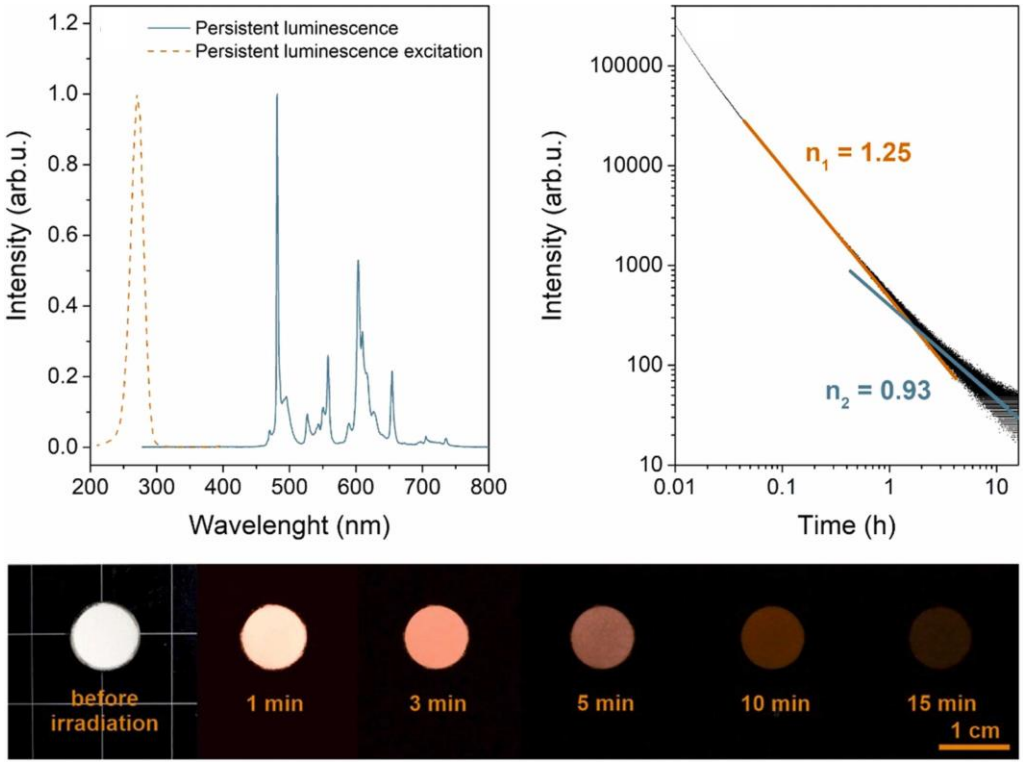
Garnet-based materials are widely investigated for applications in optics. In this study, we report the structure and spectroscopic properties of novel $Mg_3Lu_2Ge_3O_{12}:Pr^{3+}$ garnet that exhibits orange persistent luminescence. Persistent luminescence, also known as persistent phosphorescence, long-lasting phosphorescence, and long afterglow, is an optical phenomenon in which a material emits light for a prolonged time after the excitation source is turned off. The atomic positions of $Mg_3Lu_2Ge_3O_{12}$ were calculated using Rietveld refinement. The local structure analysis using extended X-ray absorption fine structure (EXAFS) and site-selective spectroscopy revealed that activator ions predominantly incorporate in the Lu^{3+} position. The persistent luminescence processes in $Mg_3Lu_2Ge_3O_{12}:Pr^{3+}$ were analysed using photoluminescence (PL), thermostimulated luminescence (TSL), and electron paramagnetic resonance (EPR) spectroscopy methods. The comparison of PL and persistent luminescence spectra implies that electron and hole traps are filled due to the photoionization of Pr^{3+} ions. Two paramagnetic defects related to O^- sites were detected after the excitation. TSL analysis indicates a quasi-continuous charge trap distribution ranging from 0.57 to 1.51 eV in the investigated host, enabling efficient persistent luminescence. The persistent luminescence mechanism of $Mg_3Lu_2Ge_3O_{12}:Pr^{3+}$ is proposed.



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The influence of Sb doping on the local structure and disorder in thermoelectric ZnO:Sb thin films

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Thermoelectric transparent ZnO:Sb thin films were deposited by magnetron sputtering, with Sb content varying between 2 and 14 at%. The films crystallize in the ZnO wurtzite structure for lower levels of Sb-doping, developing a degree of amorphization for higher levels of Sb-doping. X-ray absorption spectroscopy studies were performed to shed light on the influence of Sb doping on the local structure and disorder in the ZnO:Sb thin films. The analysis of the Zn K-edge EXAFS spectra by the reverse Monte Carlo method suggests that the introduction of Sb to the ZnO matrix promotes static disorder, which leads to partial amorphization with very small crystallites (∼3 nm) for large (12–14 at%) Sb content. Rutherford backscattering spectrometry (RBS) enabled the determination of the in-depth atomic composition profiles of the films. The film composition at the surfaces determined by X-ray photoelectron spectroscopy (XPS) matches that of the bulk determined by RBS, except for higher Sb-doping in ZnO films, where the concentration of oxygen determined by XPS is smaller near the surface, possibly due to the formation of oxygen vacancies that lead to an increase in electrical conductivity. Traces of Sb–Sb metal bonds were found by XPS for the sample with the highest level of Sb-doping. Time-of-flight secondary ion mass spectrometry obtained an Sb/Zn ratio that follows that of the film bulk determined by RBS, although Sb is not always homogeneous, with samples with smaller Sb content showing a larger Sb content closer to the film/substrate interface. From the optical transmittance and reflectance curves, it was determined that the films with the lower amount of Sb doping have larger optical band-gaps, in the range of 2.9–3.2 eV, while the partially amorphous films with higher Sb content have smaller band-gaps in the range of 1.6–2.1 eV. Albeit the short-range crystalline order (∼3 nm), the film with 12 at% of Sb has the highest absolute Seebeck coefficient (∼56 μV/K) and a corresponding thermoelectric power factor of ∼0.2 $\mu W \cdot K^{-2} \cdot m^{-1}$.

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Variation of Nonlinear Refraction and Three-Photon Absorption of Indium–Tin Oxide Quantum Dot Thin Films and Solutions in Near Infrared Range

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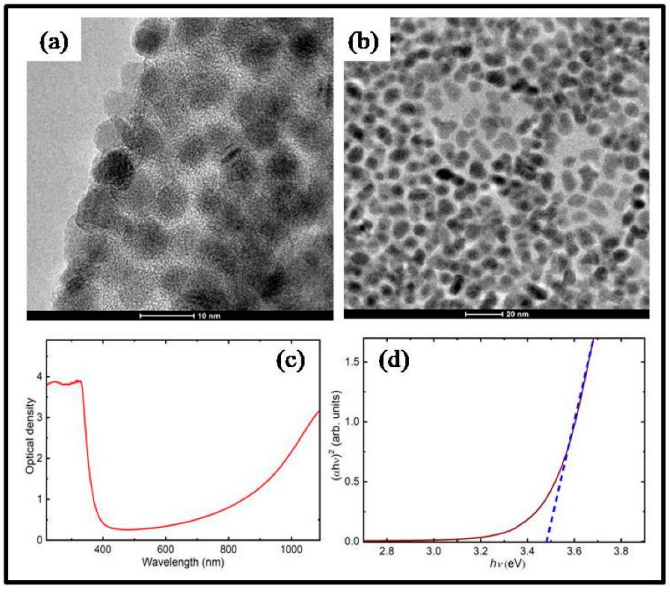
The interest in small-sized structures is due to their potential application in various fields of science such as, in particular, nonlinear optics. We characterize the nonlinear optical properties of indium–tin oxide (ITO) quantum dots (QDs) in the IR range using the Z-scan method. We present results of three-photon absorption (3PA), third harmonic generation (3HG), and Kerr-effect-induced nonlinear refraction in ITO QDs. Z-scan measurements were carried out for the QDs solution, while 3HG was demonstrated using QD thin films. The Kerr-induced nonlinear refractive index was analyzed along the 800–950 nm range showing an increase in this parameter from -6.7×10^{-18} to -1.5×10^{-17} m^2 W^{-1}. At longer wavelengths (1000–1100 nm), the higher-order effects started to contribute to a nonlinear refractive index. The 3PA coefficient at 950 nm was measured to be 1.42×10^{-25} m^3/W^2. We discuss the peculiarities in the wavelength-dependent variation of the coefficient of nonlinear absorption responsible for 3PA in the range of 800–1150 nm. Third harmonic generation was analyzed in the 1200–1550 nm spectral range. The absolute value of 3HG conversion efficiency in the 150 nm thick film at the wavelength of laser radiation (1350 nm) was estimated to be ~10^{-5}.



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Graphene Hybrid Metasurfaces for Mid-Infrared Molecular Sensors

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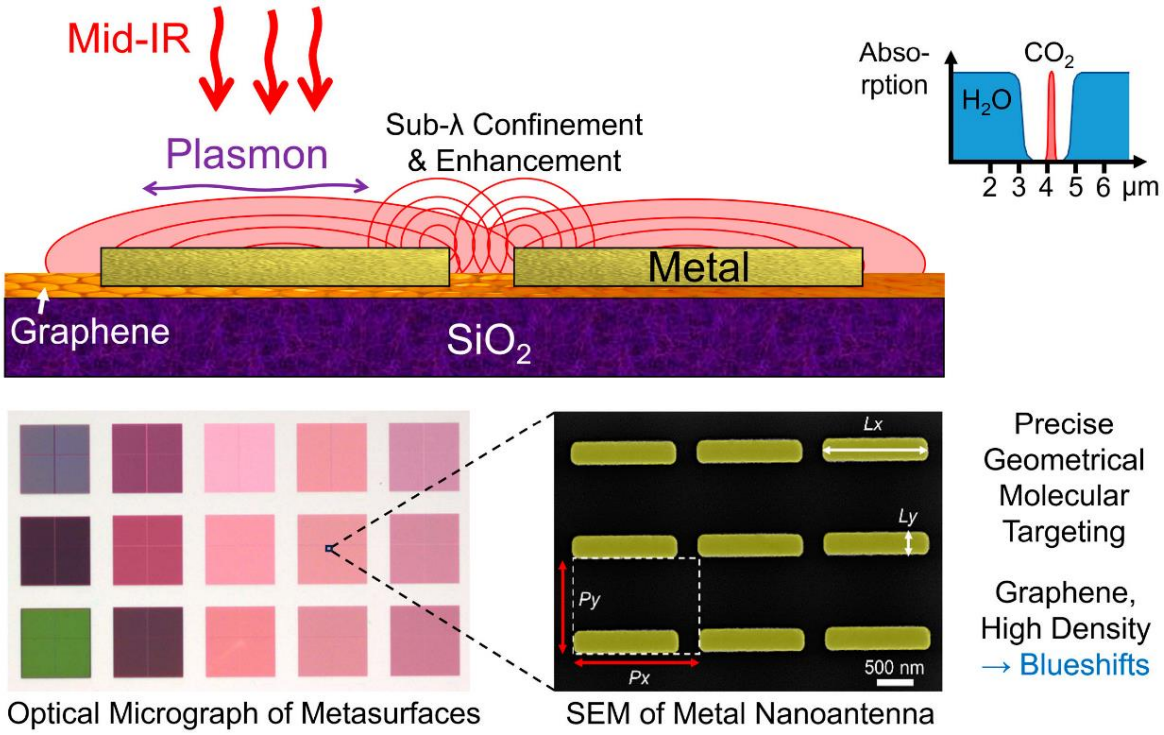
Distinctive mid-infrared (MIR) molecular vibrations, ranging between ~2 and 12 µm, act as characteristic 'molecular fingerprints' for label-free identification of a wide range of chemicals and biomolecules. Usefully, atmospheric transparency windows, at 3–5 µm and 8–13 µm, enable a range of applications such as CO2 gas sensing and alcohol detection. Within the same MIR spectral range, black body radiation can also be utilised for photodetection and thermal imaging technologies. Taken together, MIR technologies have a substantial role in environmental monitoring, medical diagnosis, and security. However, in comparison to other wavelength regions, there exists a relative lack of MIR sources, detectors, and methodologies. We integrated graphene with asymmetric metal metasurfaces and optimised the geometry-dependent photoresponse towards optoelectronic molecular sensor devices. Through careful tuning and characterisation, combining finite-difference time-domain simulations, electron-beam lithography-based nanofabrication, and micro-Fourier transform infrared spectroscopy, we achieved precise control over the mid-infrared peak response wavelengths, transmittance, and reflectance. Our methods enabled simple, reproducible and targeted mid-infrared molecular sensing over a wide range of geometrical parameters. With ultimate minimization potential down to atomic thicknesses and a diverse range of complimentary nanomaterial combinations, we anticipate a high impact potential of these technologies for environmental monitoring, threat detection, and point-of-care diagnostics.



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Chemical composition of $Na_{0.5}Bi_{0.5}TiO_3$ solid solutions with $Sr_{0.7}Bi_{0.2}TiO_3$ on a local level

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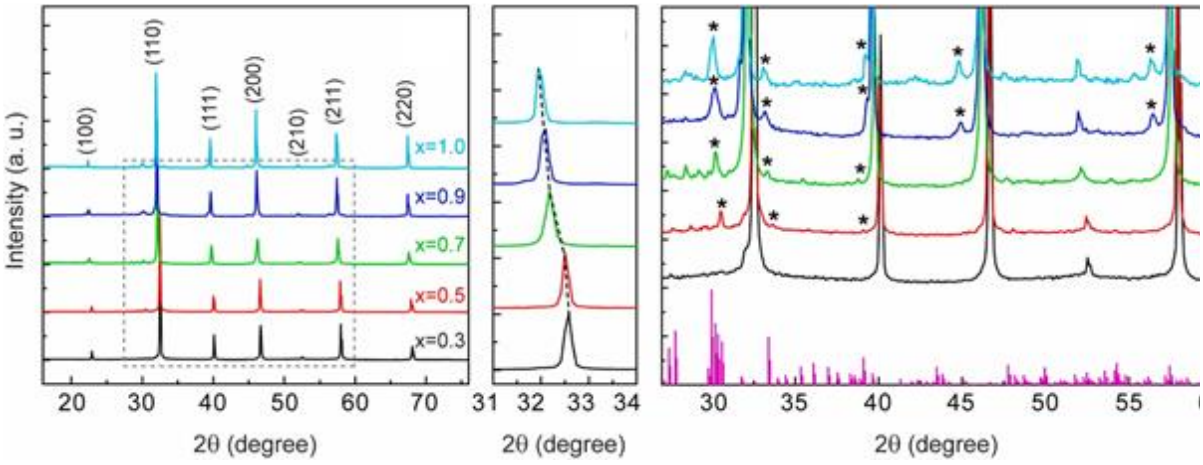
Ferroelectric properties are sensitive to defects either intentionally or unintentionally present in ferroelectric materials. Oxygen vacancies in $Na_{0.5}Bi_{0.5}TiO_3$ are of high demand as they stimulate the ionic conductivity essential to solid fuel cell applications. However, their available concentration, which is directly related to introduced A-site vacancies, is very limited. The objective of the present research is to study how the concentration of A-site vacancies may be increased by forming solid solutions with $Sr_{0.7}Bi_{0.2}TiO_3$. A thorough study of heterogeneity and chemical composition of (1-y) $Na_{0.5}Bi_{0.5}TiO_3$-y$Sr_{0.7}Bi_{0.2}TiO_3$ceramics on a local level is conducted and accompanied by impedance measurements. It is shown that the chemical composition of the matrix grains is stable and follows the designed formula, allowing the formation of A-site vacancies in a wide concentration range and, in a limited amount, also oxygen vacancies. Inclusions, the content and character of which depend on $Sr_{0.7}Bi_{0.2}TiO_3$ concentration, are detected and discussed. Complex impedance studies suggest that the compositions with y < 0.5 preserve low ionic conductivity up to 600–700 °C, but it significantly increases at higher y.



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Flexible nanosheets for plasmonic photocatalysis: microwave-assisted organic synthesis of Ni–NiO@$Ni_2CO_3(OH)_2$ core–shell@sheet hybrid nanostructures

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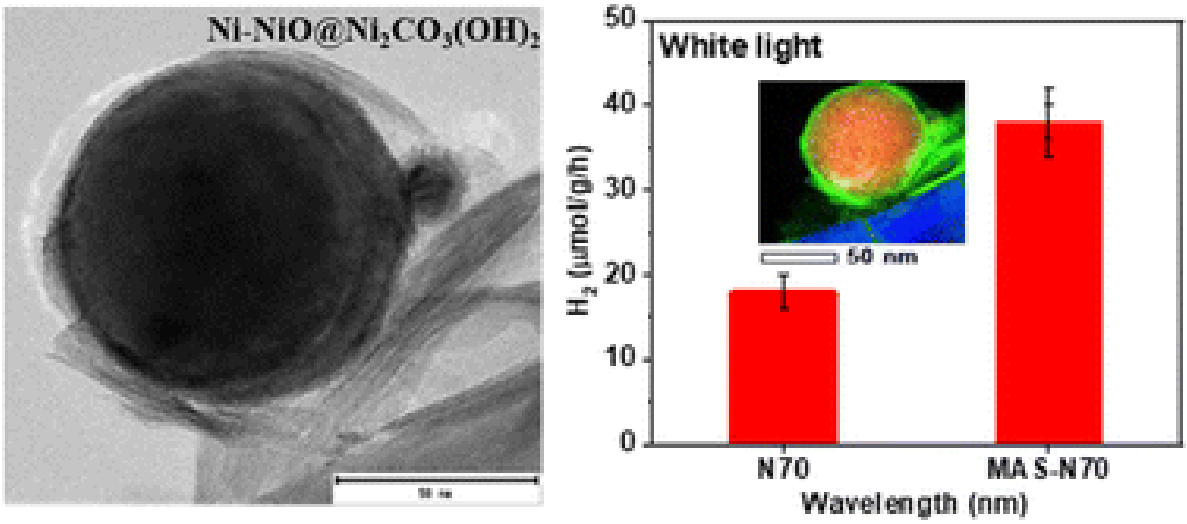
The advancement of civilization hinges upon our capacity to discover, extract, and harness energy with ever-growing proficiency. This necessity has prompted a transition from non-renewable fossil fuels to renewable energy sources. In this context, the emerging hydrogen era represents a significant stride towards a sustainable future. The production of H_2 from abundant H_2O using inexhaustible solar energy is a viable option. Visible light-active nickel-based plasmonic photocatalysts provide a cost-effective alternative to noble metals. However, their rarity, fragility, and limited understanding pose challenges.

This study presents a microwave-assisted organic synthesis of a Ni–NiO@$Ni_2CO_3(OH)_2$ core–shell@sheet plasmonic photocatalyst. By employing time and power-dependent synthesis, this catalyst exhibits flexible $Ni_2CO_3(OH)_2$ nanosheets enveloping the Ni–NiO structure, surpassing the pristine Ni@NiO/$NiCO_3$ core–shell counterpart. Chemical reaction mechanisms suggest that irradiation of pristine Ni–NiO/$NiCO_3$ nanostructures leads to breakage of amorphous $NiCO_3$ to Ni^{2+} and CO_3^{2-}, which further, in the presence of water solvent, interacts with OH^- ions leading to the formation of $Ni(CO_3)\cdot Ni(OH)_2$. With enhanced light absorption and photocatalytic properties, the resulting core–shell@sheet photocatalyst demonstrates double the hydrogen evolution reaction yield (40 µmol g^{-1} h^{-1}) compared to the pristine catalyst (20 µmol g^{-1} h^{-1}). The enhanced H2 yield is attributed to the flexible sheets, cross-dimensional photocatalyst structure, increased surface area for surface reactions, and higher H_2 activity of $Ni_2CO_3(OH)_2$. This research showcases the potential of microwave-assisted synthesis in developing flexible nanosheets with superior solar water splitting performance.



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Thermal annealing of neutron irradiation generated paramagnetic defects in transparent Al_2O_3 ceramics

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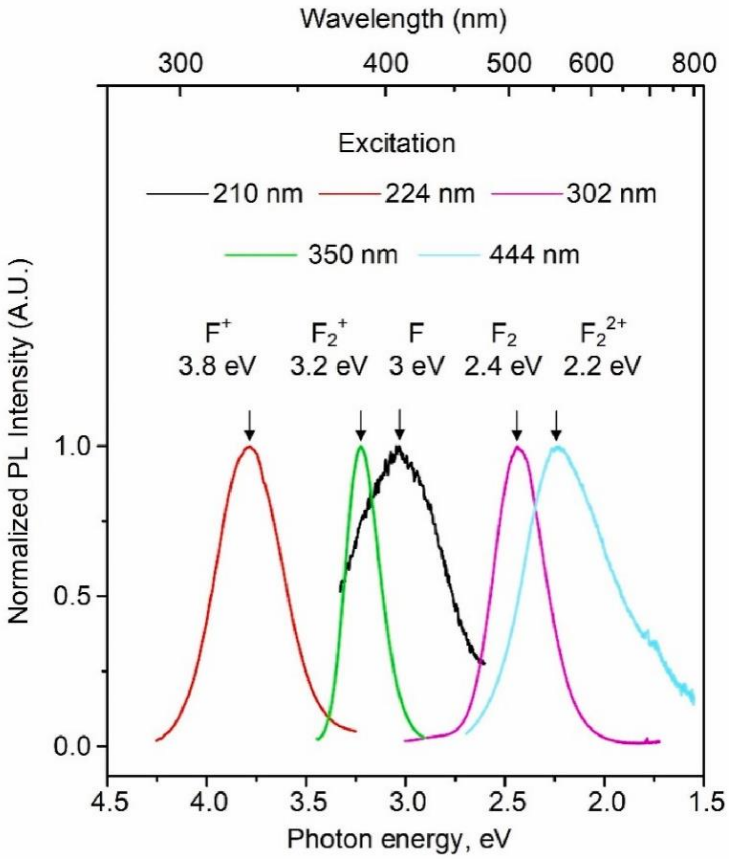
It is fundamentally important to understand, control, and predict the effect of irradiation on the structure and optical properties of functional materials. In this study, the thermal stability of fast-neutron-induced point defects has been investigated in polycrystalline transparent alumina ceramics. The results of a combined study of electron paramagnetic resonance (EPR) and photoluminescence spectroscopy are presented in this paper. The EPR signals related to different trapped-hole centers as well as electron-type F^+ centers have been observed after neutron irradiation. Rapid decay of the total EPR signal intensity occurs after annealing in the 600–750 K temperature range. The selective luminescence bands related to the F- and F_2-type centers are detected under irradiated corundum ceramics photoexcitation within relevant defect absorption bands (i.e. intracenter excitation/emission).



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Nanocrystalline $CaWO_4$ and $ZnWO_4$ Tungstates for Hybrid Organic–Inorganic X-ray Detectors

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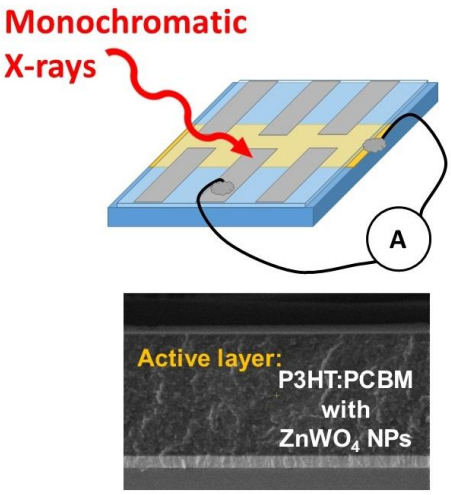
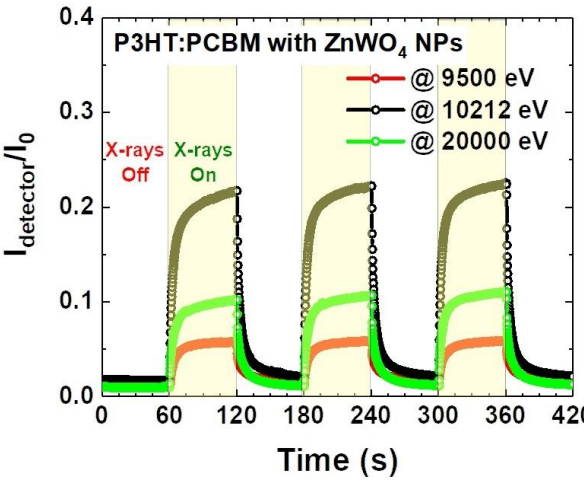
Nowadays, developing new radiation detectors based on nanomaterials is an active field of research. Hybrid materials combining an organic matrix and high-Z nanomaterials show potential for applications in radiation detection, allowing unprecedented device architectures and functionality.

In this study, novel hybrid organic–inorganic systems were produced using a mixture of tungstate ($CaWO_4$ or $ZnWO_4$) nanoparticles with a P3HT:PCBM blend. The nano-tungstates with a crystallite size of 43 nm for $CaWO_4$ and 30 nm for $ZnWO_4$ were synthesized by the hydrothermal method. Their structure and morphology were characterized by X-ray diffraction and scanning electron microscopy. The hybrid systems were used to fabricate direct conversion X-ray detectors able to operate with zero bias voltage. The detector performance was tested in a wide energy range using monochromatic synchrotron radiation. The addition of nanoparticles with high-Z elements improved the detector response to X-ray radiation compared with that of a pure organic P3HT:PCBM bulk heterojunction cell. The high dynamic range of our detector allows for recording X-ray absorption spectra, including the fine X-ray absorption structure located beyond the absorption edge. The obtained results suggest that nanocrystalline tungstates are promising candidates for application in direct organic–inorganic X-ray detectors.





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The Impact of Graphene in $Na_2FeP_2O_7$/C/Reduced Graphene Oxide Composite Cathode for Sodium-Ion Batteries

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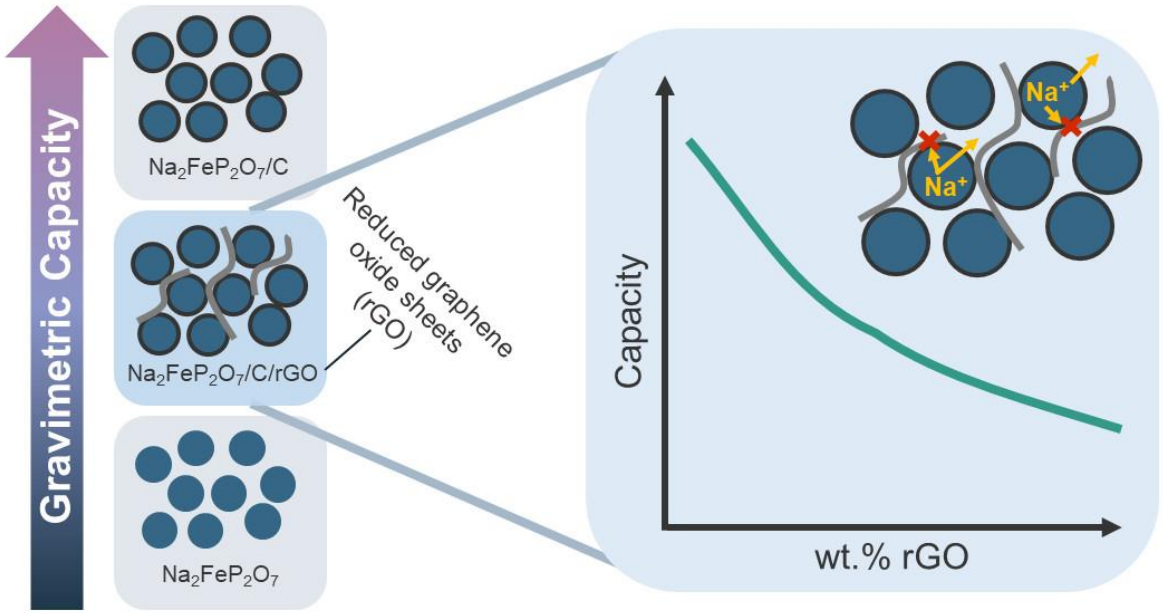
Sodium-ion batteries (SIBs) are a low-cost, safe and sustainable alternative for lithium-ion batteries (LIBs) that has over the years gained significant traction, especially when stationary, grid-level energy storage and low-cost alternatives to LIBs are concerned. While SIBs are potentially attractive LIB replacements, physicochemical differences and different material behaviors dictate that a detailed exploration and development of SIB materials are still needed.

This study presents a thorough investigation of $Na_2FeP_2O_7$ (NFP) cathode material for sodium-ion batteries and its composites with carbon and reduced graphene oxide (rGO). Our findings demonstrate that rGO sheets improve cycling performance in NFP/C/rGO composite in the absence of solid electrolyte interphase (SEI)-stabilizing additives. However, once SEI is stabilized with the help of fluoroethylene carbonate electrolyte additive, NFP with carbon additive (NFP/C) exhibits superior electrochemical performance when compared to NFP/rGO and NFP/C/rGO composites. The decreases in capacity and rate capability are proportional to the amount of rGO added, and lead to an increase in overvoltage and internal resistance. Based on our results, we attribute this effect to worsened sodium kinetics in the bulk of the electrode—the larger ionic radius of Na+ hinders charge transfer in the presence of rGO, despite the likely improved electronic conductivity. These findings provide a compelling explanation for the observed trends in electrochemical performance and suggest that the use of rGO in Na-ion battery electrodes may present challenges associated with ionic transport along and through rGO sheets.



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Theses

Doctor Theses

No.	Author	Title	Supervisor	Degree
1.	G. Doķe	Red and Near Infra-red Persistent Luminescence of Transition Metal Activated Germanate Materials	Dr. phys. Anatolijs Šarakovskis	Ph.D.
2.	A. Platoņenko	Modeling and characterization of radiation point defects in α-Al_2O_3 and $MgAl_2O_4$ crystals from first principles	Dr. rer. nat. Deniss Grjaznovs	Ph.D.
3.	M. Ķemere	Rare earth ion luminescence and energy transfer in diactivated oxyfluoride glasses and glass ceramics	Dr. hab. phys. Uldis Rogulis	Ph.D.
4.	A. Česnokovs	The effect of point defects and their local structure on the conductivity of wide-gap materials: cases of CeO_2 and ZnO	Dr. rer. nat. Deniss Grjaznovs	Ph.D.

M.Sc. Theses

No.	Author	Title	Supervisor	Study programme
1.	S. Homiča	Effect of structure of ionic liquids on conductivity for use in sodium ion batteries	Dr.chem. Guntars Vaivars	Chemistry
2.	M. Dille	Hydrothermal synthesis of copper-doped zinc sulfide materials	Mg. Katrina Laganovska, Dr. phys. Krišjānis Šmits	Chemistry
3.	M. A. Zommere	Research of original organometallic complexes of iridium and their application in light emitting diodes	Asoc. prof. Dr. phys. Aivars Vembris	Physics
4.	V.Paramonova	Reproducibility studies of the synthesis of silver nanoprisms	Asoc. prof. Dr. phys. Aivars Vembris	Chemistry
5.	L. Dipāne	Synthesis of functional one-dimensional core-shell heterostructures via metal oxide based nanowire selenization	Ph.D. Edgars Butanovs	Chemistry
6.	I. Darja	The effect of ambient illuminance on retinal illuminance	Dr. phys. Sergejs Fomis	Optometry

7.	A. Podelinska	Vibration spectroscopy of radiation resistant ceramics for fusion applications	Dr. phys. Anatolijs Popovs	Physics

B.Sc. Thesis

No.	Author	Title	Supervisor	Study programme
1.	G. Paidere	Development of microfluidic device for extracellular vesicle separation from large-volume samples	Dr. sc. ing. Roberts Rimša	Chemical technology
2.	A. Spustaka	Use of mechanoluminescence in mechanical stress mapping	Dr.phys. Virginija Vītola	Physics
3.	A. Mauručaite	The optical properties of low molecular weight compounds based on carbazole group with pyridinium ion and their use in light-emitting electrochemical cells	Asoc. prof. Dr. phys. Aivars Vembris	Physics
4.	Ē. Dipāns	Electrical measurements of charge density wave nanomaterials at cryogenic temperatures	Ph.D. Edgars Butanovs	Physics
5.	U. Alonderis	Application of an optical phase compensating structure to reduce the disturbing effects of floating elements in the vitreous body	Dr.phys. Varis Karitāns	Optometry
6.	A. Dārzniece	Application of digital signal processors in measuring optical aberrations	Dr.phys. Varis Karitāns	Optometry
7.	R. Mārtiņš Kolbergs	Synthesis and optical properties of chromium and gallium activated calcium hexaaluminate	Mg. Pāvels Rodionovs	Chemistry