

**Institute of Solid State Physics
University of Latvia**



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Contents

ANNUAL REPORT	1
Contents	3
Introduction	4
Scientific Highlights	16
Science: Theory and experimental studies.	17
Technology and experimental methods.	29
Application: applied research of materials for sensors, scintillators, detectors, materials for photonics and electronics, and materials for energy harvesting and storage.	38
Publications with the authorship of ISSP UL in Web of Science and Scopus Databases	48
Theses	61
Other important news in 2021	63

Introduction

The Institute of Solid State Physics (ISSP UL) of the University of Latvia is the main materials science institute 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 legally and fiscally independent organization of the University.

In the 1990ies, after gaining independence and before joining the EU, the funding of science in Latvia decreased/went in a free plunge, as the former sources disappeared, and new funding channels were not yet established. Under these conditions, many research institutions collapsed, and only a few strongest survived, ISSP UL among them. Four laboratories from the Institute of Physics of the Latvian Academy of Sciences joined ISSP UL in 1995. Twenty scientists of the former Nuclear Research Centre found a shelter in the ISSP UL in 1999 and established the Laboratory of Radiation Physics. In 2004 scientists from the Institute of Physical Energetics joined ISSP UL and established the Laboratory of Organic Materials.

To encourage more students to select material physics and chemistry, in mid-90ies ISSP UL stepped-up its teaching activities. Several researchers were elected as professors of the University of Latvia. Post-graduate and graduate curricula were prepared. Presently they are offered in solid-state physics, material 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 3 years 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. The Institute is involved in theoretical modelling as well as in the experimental characterization of fusion reactor construction and functional materials and has expertise in material erosion and re-deposition diagnostics in Plasma-Facing Components using Laser-Induced Breakdown Spectroscopy. 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 Horizon 2020 Teaming project: “**The Excellence Centre of Advanced Material Research and Technology Transfer – CAMART²**”. 169 proposals were submitted; 31 were selected to develop their Business Plans. The project scored 14.5 from 15 points; it was the only project from Latvia and Baltic countries. It was submitted in cooperation with Swedish partners from the Royal Institute of Technology (KTH) and the Research Institute of Sweden (RISE). During 12 months of Phase 1, a Business Plan for the future Centre of Excellence CAMART² was elaborated, demonstrating the long-term science and innovation development strategy. Its vision is to upgrade and further consolidate the ISSP UL as a key centre of excellence for education, science, innovation, and technology transfer in the Baltic countries.

The Business Plan was highly estimated in the second phase of the Horizon 2020 Teaming project, dedicated to the development of the Centre of Excellence during 2017-2023 (Figure 1).

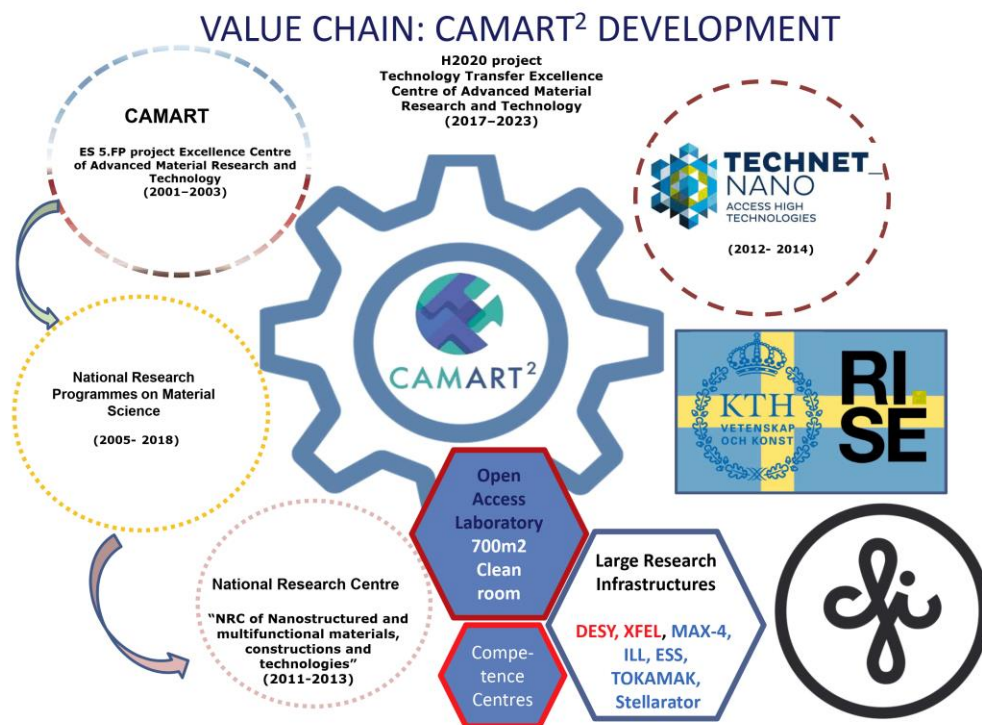


Figure 1: Value chain: CAMART² development.

ISSP UL has developed strong research and innovation ecosystem.

680 m² of ISO class 7-8 **cleanroom facility** is established, including equipment for:

- basic technological methods: thin-film fabrication and parameter control, chemical synthesis, nano-structuring;
- analytical methods: XRD analysis, electron microscopy (SEM, TEM), X-ray photoelectron spectroscopy (XPS), morphology analysis, optical and EPR spectroscopy, spectral ellipsometry;
- prototyping of photonic and electronic devices. A new dedicated prototyping cleanroom laboratory was newly established.

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 programme in physics is in progress to make it relevant to the projected industrial needs. Similar upgrades are also planned for the University's doctoral programme.

The ISSP UL aims to improve and enhance collaboration with industry in Latvia and abroad. To achieve this, it has set up a platform intended to serve as a single point of contact for scientists and companies. Named "Materize", the platform provides access to the ISSP UL's expertise and resources while facilitating communication with companies to realise projects based on industry-specific standards. Current case studies include a cleanroom-based prototyping facility, organic light-emitting diodes, optical lithography, vacuum deposition of thin films and composite nanomaterials synthesis.

Every year "Materize" hosts the Deep Science Hackathons - events for idea creation. In 2020, the 5th Deep Science Hackathon took place in February with the participation of students and professionals from various Latvian universities and companies representing such countries as India, Denmark, Lithuania, Nepal and, of course, Latvia. The second Student Deep Science Hackathon took place online in October. The Hackathon's goal is 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 ISSP UL researchers actively participated in two other international Hackathons: "Photon and Neutron Science in the Baltic Sea Region" in October and "ActInSpace" in November.

The new Research Programme of ISSP UL for the period of 2021-2023-2027 includes the three research priorities 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.

An important challenge for the Institute is to translate the new knowledge coming from the fundamental research into real innovation potential, which is addressed in Research Program as new initiatives:

- Organ-on-a-chip and Lab-on-a-chip devices for biomarkers. The project addresses application in personalized and precision medicine. It is based on expertise in easy-to-use microfluidic device design and fabrication capabilities of ISSP UL for creating a novel and impactful biological study test-bed.
- Polymer photonics technology platform. This platform offers standardized polymer photonic device preparation methods to academics and the industry. This system is based on three main parts – computational simulations of photonic devices, photonic material's engineering and formation, photonic element fabrication workflow and processing of the producible photonic elements.

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 broader than 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 integrate it better in the European Research Area by heightening the involvement in joint research programs and projects with the EU Member States, especially within the Baltic Sea region.

The mid-term milestone in Research Programme for ISSP UL is January 2025, the date to complete the Teaming project CAMART², when it comes to evaluating the planned achievements in quantified Key Performance Indicators (KPI) format as well as when full sustainability of the Institute must be achieved and demonstrated.

In the year 2021, the domain concept continued to show positive results. Sixty-nine

projects were implemented. They include 2 Horizon 2020, 3 COST projects, European Agricultural Fund for Rural Development (EAFRD) project, 3 EraNet projects, EUROfusion project, 17 European Regional Development Fund (ERDF) projects, 21 Latvian Council of Science Projects, 11 Postdoctoral projects, 2 Rural support service projects, 2 EEA and Norway Grants, 1 Latvia - France Bilateral Program “OSMOZE” project, 2 Latvia-Lithuania-Taiwan joint projects, 1 Latvian-Ukrainian Bilateral Cooperation Program and 2 National Research Programs.

The structure of ISSP UL at the end of 2021 is shown in Figure 2. It promotes research and innovation by creating a service-oriented environment, fostering openness and product-oriented research.

The highest decision-making body of ISSP UL is the **Scientific Council**, consisting of 13 members elected by the employees of the Institute (Table 1). Presently, Dr.phys. D. Bocharov is the chairperson of the ISSP UL Scientific Council. The Council appoints the director and his/her deputies.

Figure 2: The organizational structure of ISSP UL in 2021

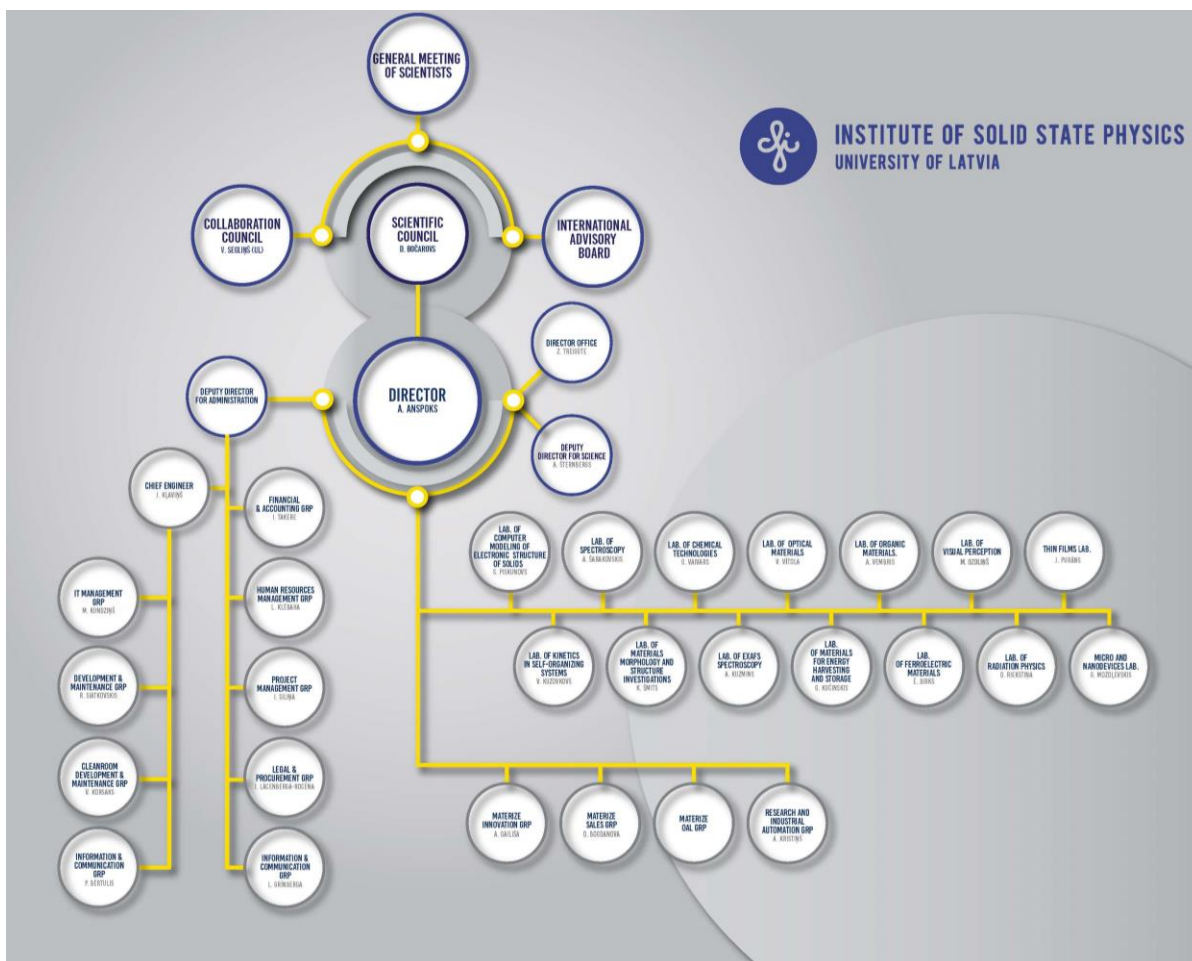


Table 1:

The Scientific Council of the Institute

1. Dmitry Bocharov, Dr.phys., Chair of the Scientific Council
2. Jeļena Butikova, Dr.phys., Vice-Chair of the Scientific Council
3. Andris Anspoks, Dr.phys., Director
4. Līga Grīnberga, Dr.phys.
5. Jurgis Grūbe, Dr.phys.
6. Sergejs Piskunovs, Dr.rer.nat.
7. Boris Polyakov, Dr.phys.
8. Kaspars Pudžs, Dr.phys.
9. Mārtiņš Rutkis, Dr.phys.
10. Anatolijs Šarakovskis, Dr.phys.
11. Andris Šternbergs, Dr.habil.phys.
12. Aivars Vembris, Dr.phys.
13. 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 (see Table 2) when making strategic decisions. Additionally, the International Advisory Board issues recommendations for the commercialization of scientific results and for improving the management.

Table 2:

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. Niels E. Christensen, Aarhus University, Denmark
6. Prof. Robert Evarestov, St. Petersburg University, Russia

7. Prof. Gunnar Niklasson, Uppsala University, Sweden
8. Prof. Dag Høvik, The Research Council of Norway, Norway
9. Prof. Marco Kirm, University of Tartu, Estonia
10. Prof. Maija Kuklja, Program director at National Science Foundation, USA
11. Dr. Jiri Kulda, Institut Laue-Langevin, France
12. Prof. Toshio Ogawa, Shizuoka Institute of Science and Technology, Japan
13. Dr. Mārtiņš Rutkis, Institute of Solid State Physics, University of Latvia, Latvia
13. Prof. Pauls Stradins, Colorado School of Mines, USA
14. Prof. Vladimir Shur, Institute of Natural Science, Ural Federal University, Russia
15. Prof. Andrejs Silins, Latvian Academy of Sciences, Latvia
16. Prof. Sergey Tiutiunnikov, Joint Institute for Nuclear Research, Russia
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. At the end of 2021, 355 employees were working at the Institute (316 employees at the end of 2020). ISSP UL research staff dynamics are shown in Figure 4, indicating an impressive increase in the number of students involved in the implementation of projects during the last two years.

This Annual Report summarizes the research activities of the ISSP UL in 2021. The KPIs of ISSP UL are reported in Table 3 below.

A list of the most significant achievements in 2021 rightfully opens the monograph by Dr.habil.phys. Anatoly Trukhin on “Silicon Dioxide and the Luminescence of Related Materials: Crystal Polymorphism and the Glass State” published by Cambridge Scholars Publishing. This book is devoted to studying the properties of materials that can be in the crystalline and glassy state with a central focus on the physics of solids, the structure of which is disordered.

Totally 122 papers were published in peer-review journals (16 papers are still in press and will appear in 2022). Fifty-nine of them (48%) were published in the journals with the SNIP factor >1 (compared to 40% in 2020). For the first time, the average SNIP per publication (1.04) was larger than 1.

It is necessary to separately note the publication of the first article in the Nature Communications journal (doi: 10.1038/s41467-021-21991-x). This comprehensive study was performed by a collaboration between seven international laboratories with a significant

contribution from the ISSP team. It was devoted to YH_3 under pressure up to 180 GPa and will contribute to a better understanding of high-temperature superconductivity in metal hydrides.

Several metrics, as provided by the SCOPUS database, were used to evaluate the research output of ISSP and its change during the last six years (2016-2021). 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 publications are among the most-cited ones within the entire Scopus database or have been published in the most-cited journals indexed by Scopus. One of the noticeable achievements during 2021 was a significant increase from 11% in 2020 to 21% in 2021 (Figure 5) in the percent of ISSP publications that are among the top 10% of most cited publications worldwide. The percent of publications in the top 10% of the most-cited journals indexed by Scopus increased from 16% in 2020 to 23% in 2021 (Figure 6).

The third metric, Field-Weighted Citation Impact (FWCI), measures how citations received by ISSP publications compare to the world average. An FWCI value of 1.00 indicates that the entity's publications were cited exactly as expected based on the global average of similar publications. The FWCI of ISSP publications for the first time was above one (1.13) compared to the world average, indicating an increase in the publication quality (Figure 7).

The fourth metric shows the distribution of ISSP publications across journals, divided into four quartiles according to their Impact Factor. It is important to stress that about 81% (67% in 2020) of all publications 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 Ph.D. levels. In 2021, 1 Ph.D., 8 M.Sc. and 12 B.Sc theses were prepared and successfully defended.

The high quality of the research at ISSP UL was recognized by the Latvian Academy of Sciences (LAS). Two studies conducted by the ISSP teams were among the winners of the Science Achievements Competition 2021. The study on "The influence of the local atomic structure of molybdates and tungstates on their thermochromic and magnetic properties" was among the best achievements in theoretical science, whereas the study on "An innovative, high-speed Thermo-Electric Radiation Sensor (TESS)" was among the best achievements in applied science. A

collaboration between the Riga Technical University, Latvian Institute of Organic Synthesis, Institute of Solid State Physics University of Latvia, Latvian Biomedical Research and Study Centre, Rīga Stradiņš University, Institute of Atomic Physics and Spectroscopy University of Latvia, Rēzekne Academy of Technologies, Latvian State Institute of Wood Chemistry, Institute of Electronics and Computer Science on the topic “Integration of reliable technologies for protection against Covid-19 in healthcare and high-risk areas” was acknowledged with the Diploma of the LAS.

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

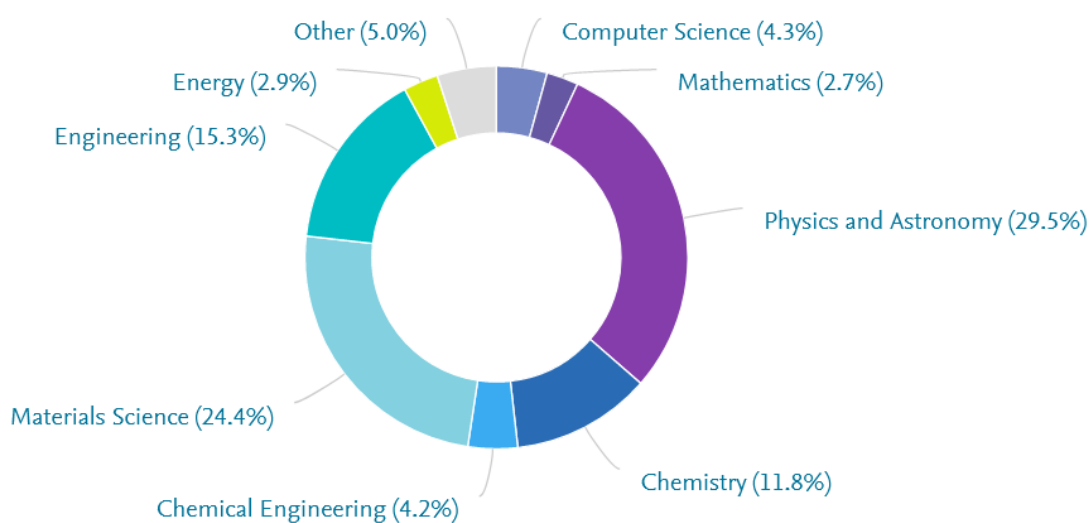


Figure 4: ISSP UL research staff dynamics 2009-2021

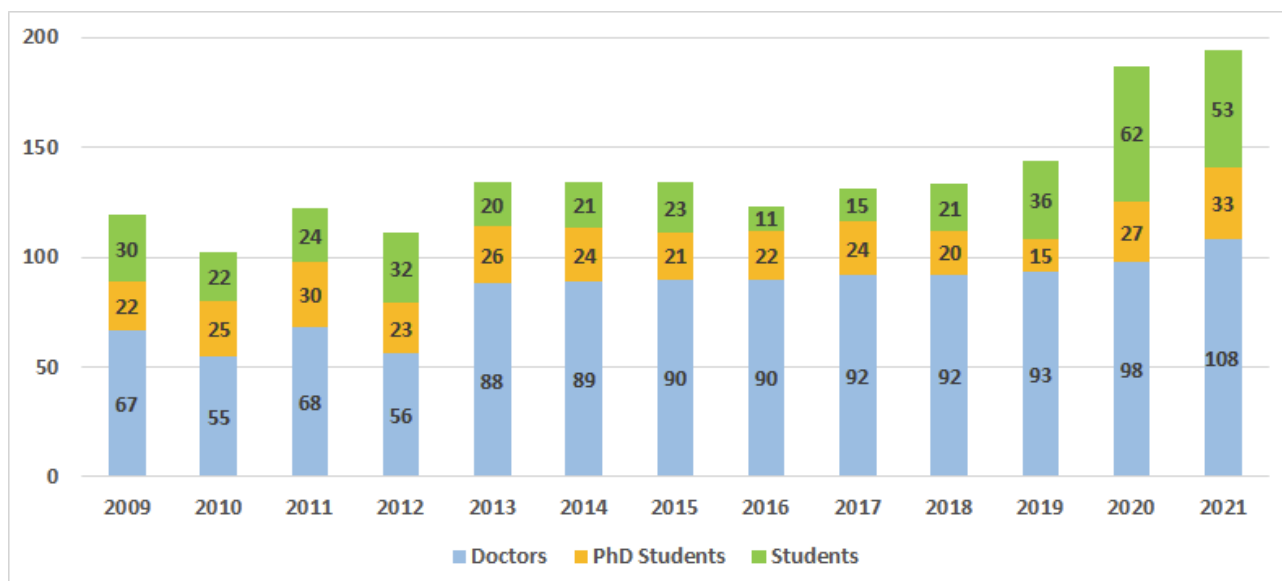


Figure 5: Share of the ISSP UL publications belonging to the top 10% of most cited publications worldwide (from Scopus database)

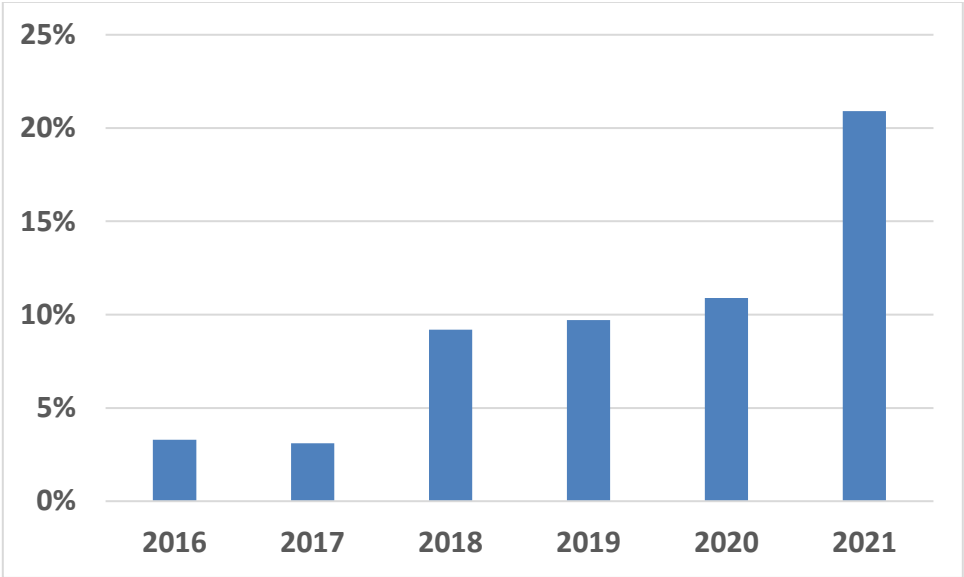


Figure 6: Share of the ISSP UL publications belonging to the top 10% of the most-cited journals indexed by Scopus (from Scopus database)

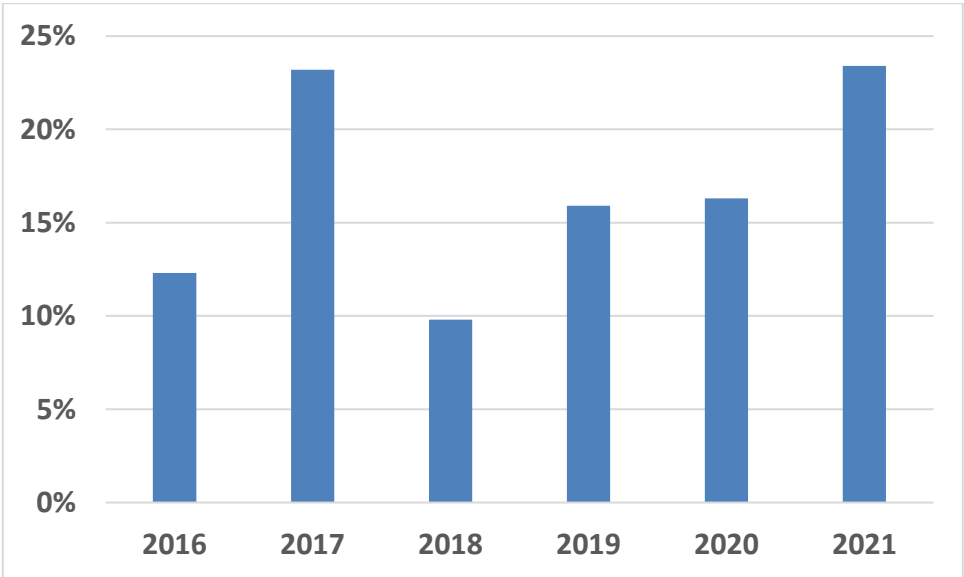


Figure 7: Field-Weighted Citation Impact (FWCI) of ISSP UL publications compared with the world average. An FWCI of 1.00 indicates that the ISSP UL publications have been cited exactly as would be expected based on the global average for similar publications (from the Scopus database)

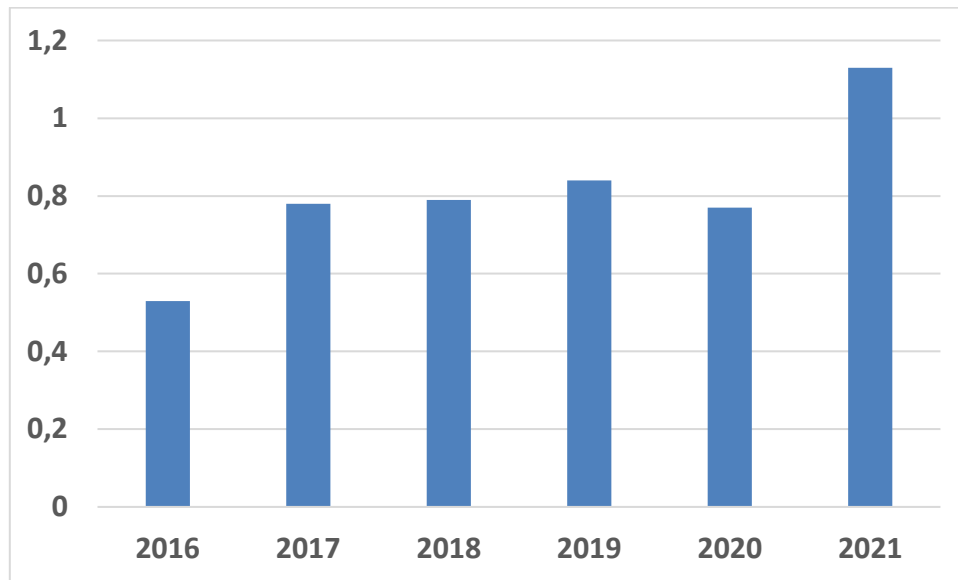


Figure 8: ISSP UL publications by Journal quartile (from Scopus database)

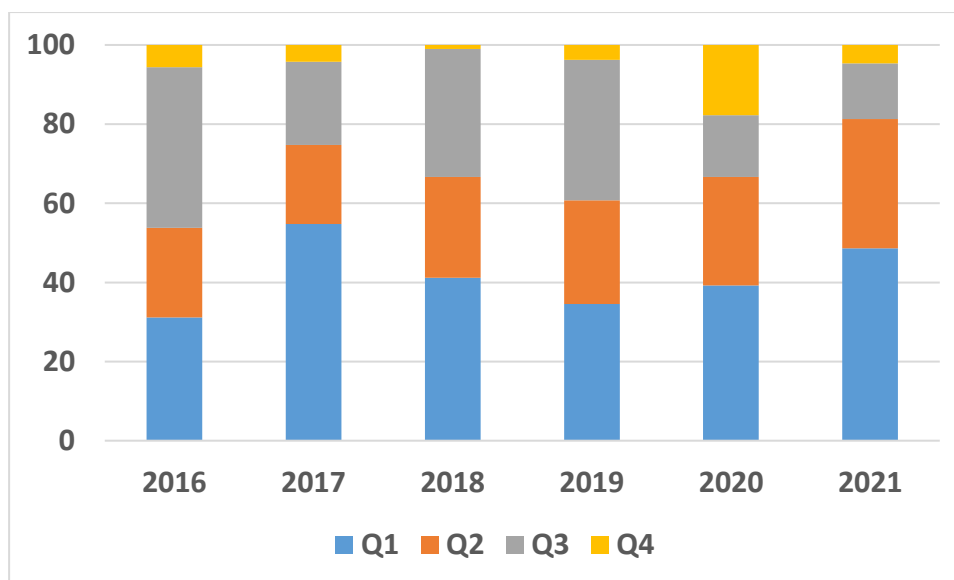


Table 3:

Key performance indicators

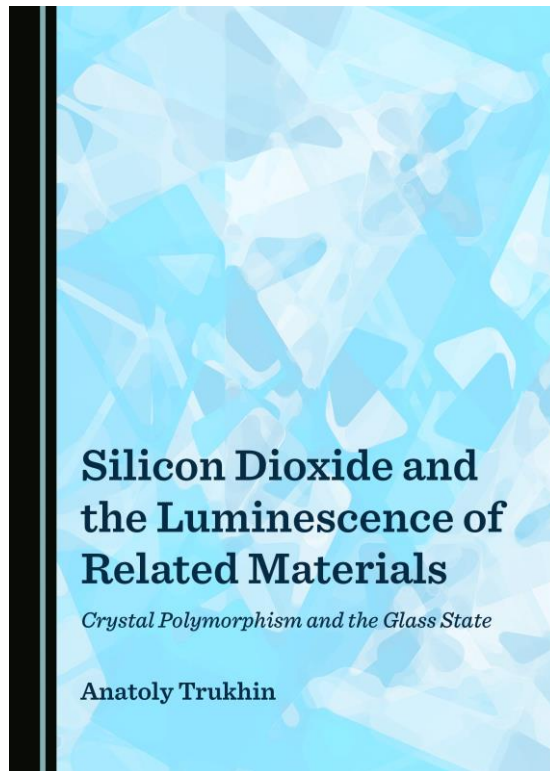
Key performance indicators for Research	3 years average (2015-2017)	2018	2019 (Mid-CAMART ²)	2020	2021	2024 (End of CAMART ²)	2026 (Sustainability)
Number of scientific publications according to "Scopus"	119	129	120	127	122 (+16)	300	400
A fraction of scientific publications in Int. Collaboration (%)	62	66	57	78	73	60	65
Number of citations/year according to "Scopus"	2170	2233	2440	3312	2665	2 500	5 000
Average SNIP per publication	0.811	0.875	0.908	0.948	1.04	1.100	1.250
Number of scientific and technical personnel (FTE)	112	126	124	138	145	170	180
Publications/FTE	0.92	1.02	0.97	0.92	0.84	1.76	2.22
Gender balance of scientific and technical personnel (% female)	24	27.2	31	30	31	33	37

Scientific Highlights

Silicon Dioxide and the Luminescence of Related Materials: Crystal Polymorphism and the Glass State

by Anatoly Trukhin

The book describes the properties of materials that can be in a crystalline and glassy state with the main focus on the physics of solids, whose structure is disordered. The approach used in the book is based on a comparison of data for crystals and glasses formed by the same atoms, with special attention to poorly studied glass-forming crystals.



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Science: Theory and experimental studies.



Local electronic structure rearrangements and strong anharmonicity in YH₃ under pressures up to 180 GPa

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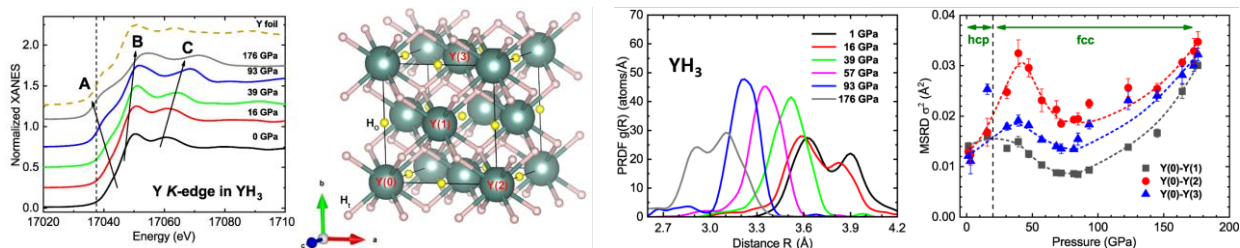
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The discovery of superconductivity above 250 K at high pressure in LaH₁₀ and the prediction of overcoming the room temperature threshold for superconductivity in YH₁₀ urge for a better understanding of hydrogen interaction mechanisms with the heavy atom sublattice in metal hydrides under high pressure at the atomic scale.

In this study, we used locally sensitive X-ray absorption fine structure spectroscopy (XAFS) to get insight into the nature of phase transitions and the rearrangements of local electronic and crystal structure in archetypal metal hydride YH₃ under pressure up to 180 GPa. The combination of the experimental methods allowed us to implement a multiscale length study of YH₃: XAFS (short-range), Raman scattering (medium-range) and XRD (long-range). XANES data evidence a strong effect of hydrogen on the density of 4d yttrium states that increases with pressure and EXAFS data evidence a strong anharmonicity, manifested as yttrium atom vibrations in a double-well potential.



Pressure-dependent Y K-edge XANES spectra of YH₃. The XANES of yttrium foil at normal pressure (dashed line) is shown for comparison, and the position of its edge is indicated by the vertical dashed line. The crystal structure of the fcc YH₃ phase is shown at the right.

Pressure dependences of the pair radial distribution functions (PRDFs) for the first Y(0)-Y(1) shell and the mean square relative displacements (MSRDs) σ² for the three nearest Y-Y shells around Y(0) atoms in the hcp and fcc YH₃ phases.

Published in

J. Purans, A. P. Menushenkov, S. P. Besedin, A. A. Ivanov, V. S. Minkov, I. Pudza, A. Kuzmin, K. V. Klementiev, S. Pascarelli, O. Mathon, A. D. Rosa, T. Irifune, M. I. Eremets, Local electronic structure rearrangements and strong anharmonicity in YH₃ under pressures up to 180 GPa, *Nat. Commun.* **12** (2021) 1765, doi: 10.1038/s41467-021-21991-x.

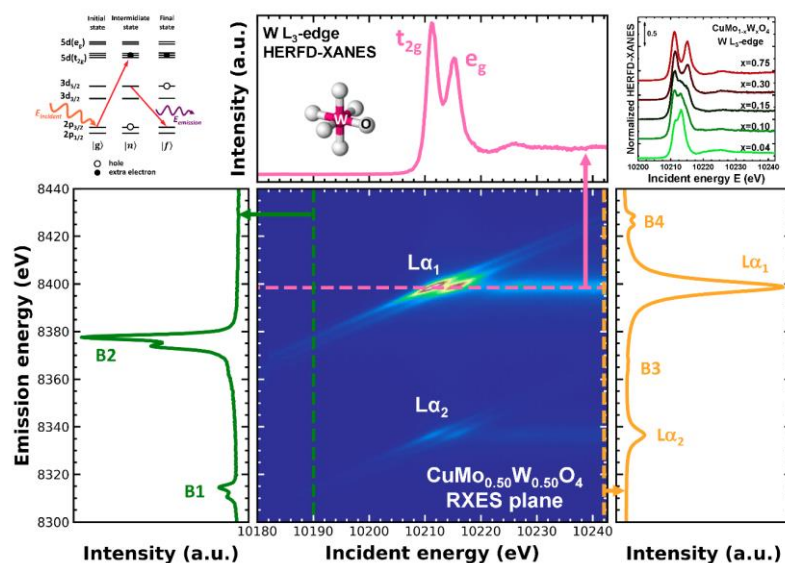
Study of the thermochromic phase transition in $\text{CuMo}_{1-x}\text{W}_x\text{O}_4$ solid solutions at the W L_3 -edge by resonant X-ray emission spectroscopy

I. Pudza, A. Kalinko, A. Cintins, A. Kuzmin

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A series of $\text{CuMo}_{1-x}\text{W}_x\text{O}_4$ solid solutions represent a group of functional materials, which demonstrate a wide range of remarkable physical and chemical properties, including thermochromic, piezochromic, halochromic and thermosensitive.

In this work, they were studied by the resonant X-ray emission spectroscopy (RXES) at the W L_3 -edge to follow a variation of the tungsten local atomic and electronic structures across thermochromic phase transition as a function of sample composition and temperature. The experimental results were interpreted using ab initio calculations. The crystal-field splitting parameter Δ for the 5d(W)-states was obtained from the analysis of the RXES plane and was used to evaluate the coordination of tungsten atoms. Temperature-dependent RXES measurements were successfully employed to determine the hysteretic behaviour of the structural phase transition between the α and γ phases in $\text{CuMo}_{1-x}\text{W}_x\text{O}_4$ solid solutions on cooling and heating, even at low ($x < 0.10$) tungsten content.



Top row: A schematic diagram of the 2p3d RXES process for octahedral tungsten coordination showing initial, intermediate and final states (left panel). The W L_3 -edge HERFD-XANES spectrum measured at the emission energy $E_e = 8398.5$ eV, indicated by the horizontal dashed line in the RXES plane (central panel). Concentration dependence of the W L_3 -edge HERFD-XANES spectra for different $\text{CuMo}_{1-x}\text{W}_x\text{O}_4$ solid solutions. Bottom row: RXES intensity map as a function of incident and emitted energies for $\text{CuMo}_{0.50}\text{W}_{0.50}\text{O}_4$ solid solution.

It was found that tungsten ions have octahedral coordination for $x > 0.15$ in the whole studied temperature range (90-420 K), whereas their coordination changes from tetrahedral to octahedral upon cooling for smaller ($x \leq 0.15$) tungsten content. Nevertheless, some amount of tungsten ions was found to co-exist in the octahedral environment at room temperature for $x < 0.15$. The obtained results correlate well with the color change in these solid solutions.

Published in:

*I. Pudza, A. Kalinko, A. Cintins, A. Kuzmin, Study of the thermochromic phase transition in $\text{CuMo}_{1-x}\text{W}_x\text{O}_4$ solid solutions at the W L_3 -edge by resonant X-ray emission spectroscopy, **Acta Mater.** **205** (2021) 116581, doi: 10.1016/j.actamat.2020.116581.*

Dielectric response of BaTiO₃ electronic states under AC fields via microsecond time-resolved X-ray absorption spectroscopy

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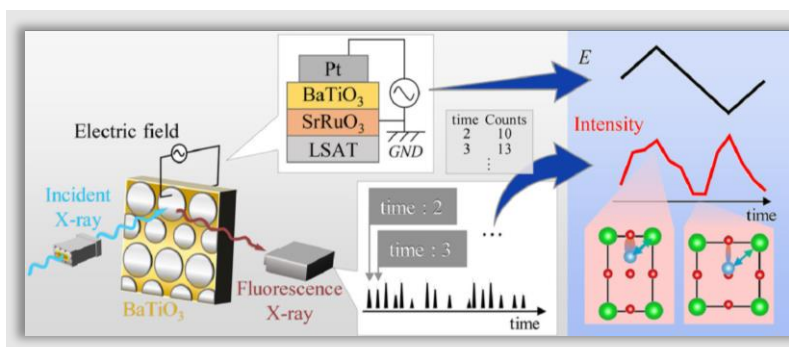
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For the first time, the dielectric response of a BaTiO₃ thin film under an AC electric field is investigated using microsecond time-resolved X-ray absorption spectroscopy at the Ti K-edge in order to clarify correlated contributions of each constituent atom on the electronic states. Intensities of the pre-edge peak and shoulder structure just below the main edge increase with an increase in the amplitude of the applied electric field, whereas that of the main peak decreases in an opposite manner. Based on the multiple scattering theory, the increase and decrease of the e_g and main peaks are simulated for different Ti off-center displacements.



Our results indicate that these spectral features reflect the inter- and intra-atomic hybridization of Ti 3d with O 2p and Ti 4p respectively. In contrast, the shoulder structure is not affected by changes in the Ti off-center displacement but is susceptible to the effect of the corner site Ba ions. This is the first experimental verification of the electronic contribution of Ba to polarization reversal.

Published in:

S. Kato, N. Nakajima, S. Yasui, S. Yasuhara, D. Fu, J. Adachi, H. Nitani, Y. Takeichi, A. Anspoks, Dielectric response of BaTiO₃ electronic states under AC fields via microsecond time-resolved X-ray absorption spectroscopy, *Acta Mater.* **207** (2021) 116681, doi: 10.1016/j.actamat.2021.116681.

Evidence of dimerization of nickel ions in NiWO₄ and Zn_cNi_{1-c}WO₄ solid solutions probed by EXAFS spectroscopy and reverse Monte Carlo simulations

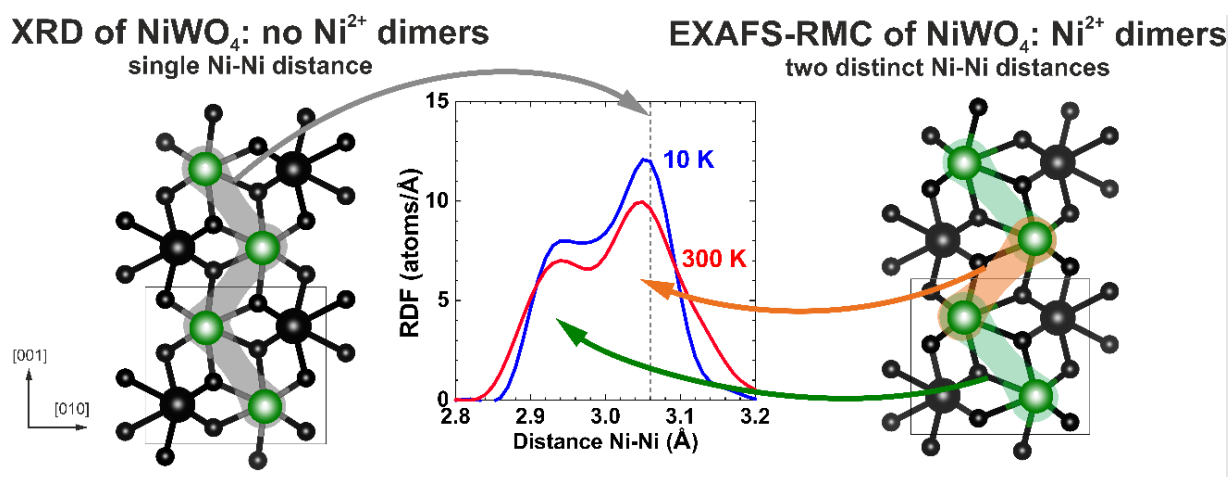
G. Bakradze, A. Kalinko, A. Kuzmin

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Magnetic properties of NiWO₄ have drawn considerable attention in the past: it is known that below the Néel temperature ($T_N=60-67$ K), the antiferromagnetic AF1-type ordering of spins prevails in bulk NiWO₄. At the same time, ZnWO₄ is a diamagnetic material, so one can expect that the dilution of nickel ions with zinc ions will affect the magnetic ordering and local interactions in Zn_cNi_{1-c}WO₄ solid solutions, thus, influencing the local structure of the compound.

In this study, the existence of exchange-coupled Ni²⁺ ions – the so-called magnetic dimers – in wolframite-type NiWO₄ and Zn_cNi_{1-c}WO₄ solid solutions with high nickel content was discovered by X-ray absorption spectroscopy combined with the reverse Monte Carlo (RMC) simulations.

Temperature (10–300 K) and composition-dependent X-ray absorption spectra were measured at the Ni K-edge, Zn K-edge, and W L₃-edge of microcrystalline NiWO₄, Zn_cNi_{1-c}WO₄ and ZnWO₄. Structural models were obtained from simultaneous analysis of the extended X-ray absorption fine structure (EXAFS) spectra at three metal absorption edges using RMC simulations. The obtained radial distribution functions for different atomic pairs made it possible to trace in detail the changes in the local environment of metal ions and the effect of thermal disorder.



Dimerization of Ni²⁺ ions within quasi-one-dimensional zigzag chains of [NiO₆] octahedra running along the c-axis directions was evidenced in NiWO₄ in the whole studied temperature range. It manifests itself as the splitting of the Ni–Ni radial distribution function into two separate peaks. The effect is further preserved in solid solutions Zn_cNi_{1-c}WO₄ for $c \leq 0.6$, which is related to the probability to find two Ni²⁺ ions in neighbouring positions.

Published in:

*G. Bakradze, A. Kalinko, A. Kuzmin, Evidence of dimerization of nickel ions in NiWO₄ and Zn_cNi_{1-c}WO₄ solid solutions probed by EXAFS spectroscopy and reverse Monte Carlo simulations, **Acta Mater.** 217 (2021) 117171, doi: 10.1016/j.actamat.2021.117171.*

Unprecedented pressure-driven metallization and topological charge transport in an anion radical salt

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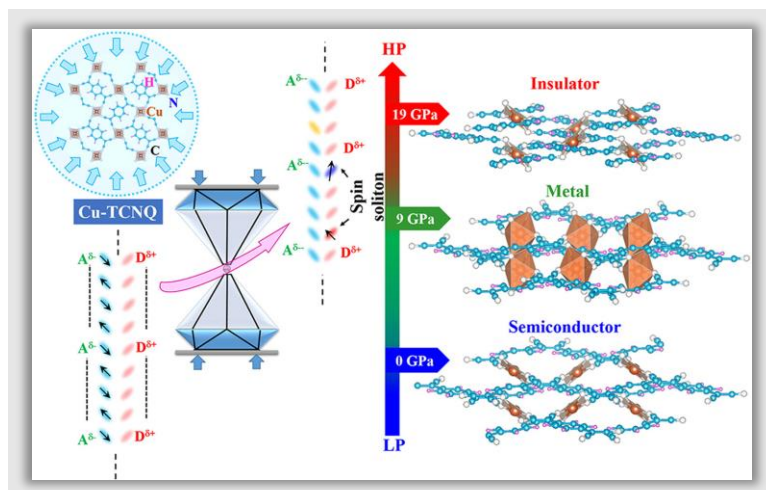
The hybrid inorganic/organic closed-stacking and soft lattice of a copper anion radical (Copper-7,7,8,8-tetracyanoquinodimethane) renders its electrical conductivity and structural modifications, which are susceptible to temperature and pressure. The geometry of its metal-ligand construction

contemplates the concept of topology with a charge-transfer instability. A pressure-induced ionic-neutral phase transition occurs and accompanies an anomalously large electrical conductivity, carries topological charges, and possesses a low energy gap smaller than the Coulomb gap. X-ray absorption spectroscopy of the metal established the high electrical conduction by the topological charges. X-ray diffraction and the first-principles calculations further suggested that the

compression leads to an irreversible alteration in the metal coordination and rotation of the quinoid rings of the anion. The present observation demonstrates a close coupling of topological charges and lattice dynamics within a relatively low-pressure regime, which may expand a novel paradigm for the comprehensive topological charge transport phenomena including thermoelectric effects in the future.

Published in:

S. Samanta, A. S. Nissimagoudar, R. Basori, A. Kuzmin, M. Li, J. Zhang, L. Wang, Y. Tian, H.-K. Mao, *Unprecedented pressure-driven metallization and topological charge transport in an anion radical salt*, **Mater. Today Phys.** **20** (2021) 100467, doi: 10.1016/j.mtphys.2021.100467.



Topological charge transport in Cu-TCNQ under pressure and three different electronic phases namely semiconducting (ambient), metallic, and insulating phases.

Metallic subnanometer porous silicon: A theoretical prediction

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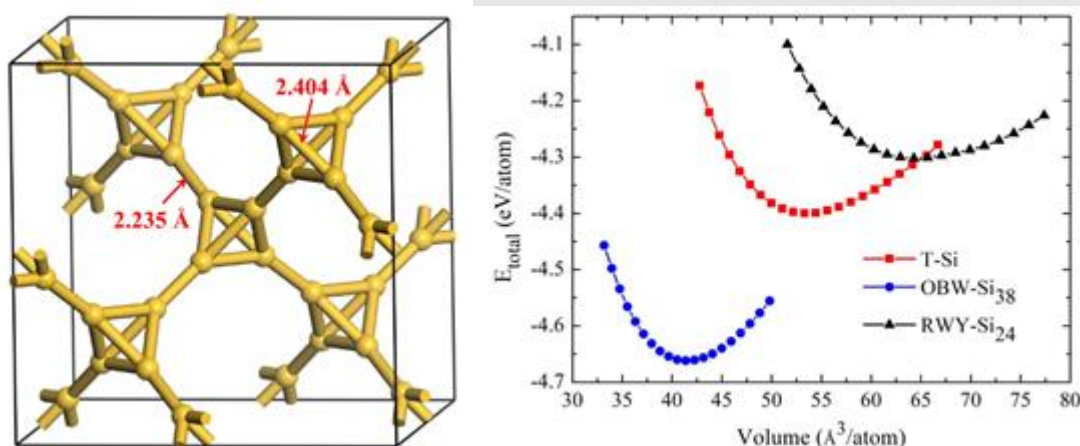
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Silicon (Si), the 14th element in the periodic table, is the second most abundant element on Earth. There are numerous silicon allotropes, in which the most stable one under normal pressure is the cubic silicon with a diamond structure (d-Si or Si-I phase).



Left panel: The cubic crystalline structure of T-silicon. Its lattice constant is 11.959 Å. The intra and intertetrahedron bond lengths are marked on the sketch in red which are 2.404 Å and 2.235 Å, respectively. Right panel: Energies per atom as functions of the volumes per atom for T-Si, OBW-Si₃₈, and RWY-Si 24 systems with relatively low densities. Note that the minima of the total energies are shifted to the corresponding cohesive energies.

In the present work, T-Si, a silicon-based counterpart of T-carbon, has been designed with the aid of density functional theory (DFT) calculations. Its stability has been fully confirmed from energetic, mechanical, lattice dynamic, and thermodynamic aspects. Due to the space extrusion, the delocalized electrons on the Si₄ tetrahedrons are squeezed onto the inter-tetrahedron Si–Si bonds, which therefore leads Ti-Si to be metallic. Furthermore, the electronic conductivity of this new material has also been predicted and discussed in this work. This new silicon allotrope with a low density of 0.869 g/cm³ can even float on water. This designed ultralight form of Si paves the way for applications in the fields of spacecraft and automobiles in the future.

Published in:

P. Fu, D.C. Yang, R. Jia, Z.J. Yi, Z.F. Liu, X. Li, R.I. Eglitis, Z.M. Su, *Metallic subnanometer porous silicon: A theoretical prediction*, *Phys. Rev. B* **103** (2021) 014117, doi: 10.1103/PhysRevB.103.014117.

Dipoles in 4,12,4-graphyne

D.C. Yang^a, Y.B. Tan^b, R.I. Eglitis^c, S. Bibi^d, R. Jia^{a,c}, H.X. Zhang^a

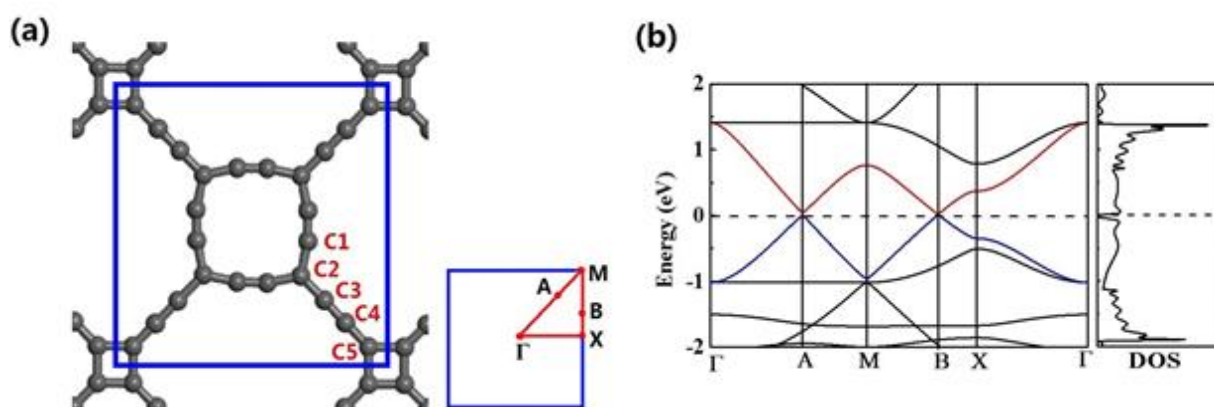
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Introducing a dipole in a neutral material can establish a localized built-in electric field, which may provide an avenue to artificially alter the electronic and optical properties of the materials. Owing to their electron configurations, boron (B) and nitrogen (N) can form a simple dipole together in a suitable lattice. Considering the atomic sizes, carbon allotropes probably are their best hosts.



(a) Sketches for 4,12,4-graphyne and its first Brillouin zone. The lattice constants are $a=b=11.07$ Å according to our simulation at PBE level. The five nonequivalent atoms are flagged out; (b) the band structure and density of states (DOS) map of the pristine 4,12,4-graphyne calculated at PBE level. Note that the Fermi level is shifted to zero.

In present work, B-N pairs as dipole source were introduced into 4,12,4-graphyne. According to the density functional theory (DFT) simulations, the electronic configurations of the doped 4,12,4-graphyne systems were significantly modified owing to the built-in electric fields caused by the B-N dipoles. Different B-N concentrations and arrangements can alter the electronic structure of 4,12,4-graphyne. Consequently, an obvious in-plane piezoelectricity can also be induced. Moreover, the direct band gap can be delicately modulated from 150 meV to 660 meV at PBE level. The B-N dipoles can also greatly enhance the light absorption instead of shifting the absorption region. According to this study, the manipulation of the dipoles in 2D carbon materials is an effective way to acquire the functional materials with some desired physical properties.

Published in:

D.C. Yang, Y.B. Tan, R.I. Eglitis, S. Bibi, R. Jia, H.X. Zhang, *Dipoles in 4,12,4-graphyne*, **Appl. Surf. Sci.** **545** (2021) 148991, doi: 10.1016/j.apsusc.2021.148991.

The local atomic structure and thermoelectric properties of Ir-doped ZnO: hybrid DFT calculations and XAS experiments

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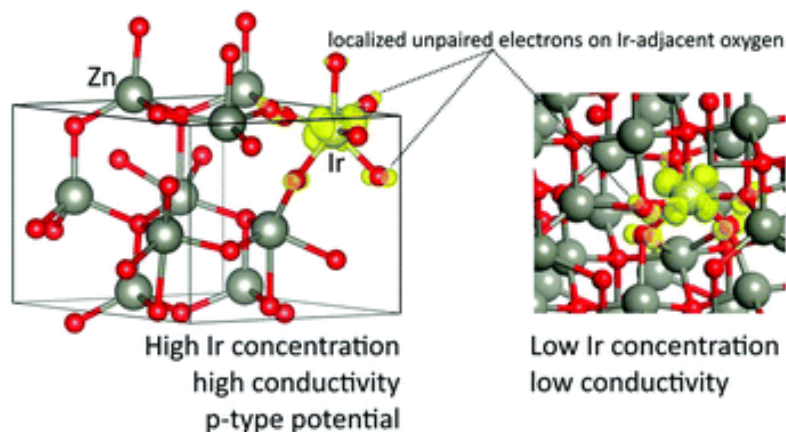
We combined the hybrid density functional theory (DFT) calculations and X-ray absorption spectroscopy (XAS) experiments in the study of the local atomic structure around Ir ions in ZnO thin films with different iridium content. This was then used in the first principles analysis of the thermoelectric properties of material. The emphasis has been put on the conditions for a positive Seebeck coefficient and p-type electrical conductivity as the functions of the Fermi level. We studied both computationally and experimentally several possible IrO_x polyhedra (complexes) with a different number of surrounding oxygens and Ir oxidation states, including those with the formation of peroxide ions (O₂²⁻). In particular, octahedral coordination of iridium ions was identified by reverse Monte Carlo (RMC) simulations of the Ir L₃-edge EXAFS spectra of ZnO:Ir thin films as the predominant complex, which is supported by the calculated lowest interstitial oxygen incorporation energies.

All the calculated IrO_x (x = 4, 5, 6) complexes, regardless of Ir the oxidation state, demonstrate potential for p-

type conduction if the Fermi level (μ_F) falls in the range of 0–0.8 eV from the valence band maximum (VBM) and the Ir concentration is high enough (12.5% in the present DFT calculations). Even though the corresponding calculated Seebeck coefficient (S) around 80–89 $\mu\text{V K}^{-1}$ slightly exceeds the experimental values, we emphasise the presence of an important plateau in the dependence of S on μ_F in this range for two complexes with the formation of peroxide ions (O₂²⁻). We predicted also that peroxide ions O₂²⁻ are characterized by the calculated phonon frequencies of 810–942 cm^{-1} in agreement with our previous Raman experimental results. In this light, we discuss the high sensitivity of calculated $S(\mu_F)$ dependences to the atomic and electronic structure.

Published in:

A. Chesnokov, D. Gryaznov, N. V. Skorodumova, E. A. Kotomin, A. Zitolo, M. Zubkins, A. Kuzmin, A. Anspoks, J. Purans, *The local atomic structure and thermoelectric properties of Ir-doped ZnO: hybrid DFT calculations and XAS experiments*, **J. Mater. Chem. C** 9 (2021) 4948-4960, doi: 10.1039/D1TC00223F.



Growth of epitaxial oxide films stabilized by oxygen vacancy dipoles

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Perovskite ABO_3 -type metal oxides possess a variety of unique properties: they exhibit electronic behavior that can range from insulator to superconductor; they display ordering of charge, magnetic spins, and/or electric dipoles; and they demonstrate strong responses to external stimuli. This rich diversity of properties enables numerous emerging and commercial applications of perovskite oxides in different sectors of electronics, photonics, and related fields.

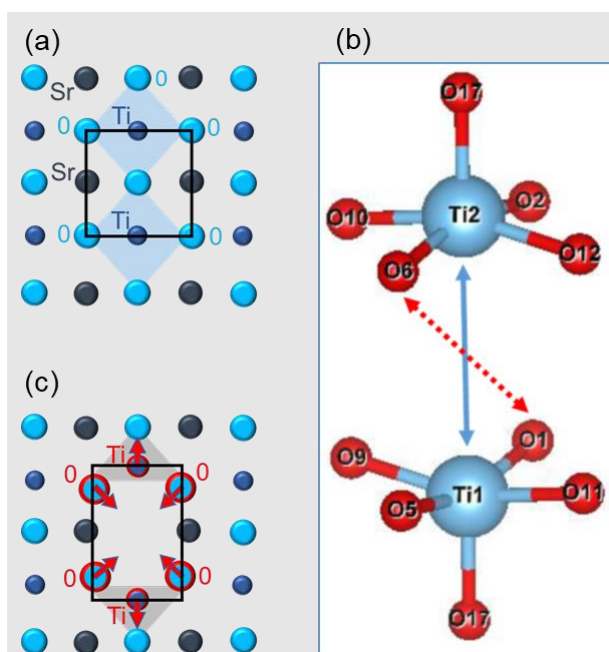
Single-crystal epitaxial films of scientifically intriguing and technologically important multifunctional ABO_3 perovskite-type metal oxides are essential for in-depth understanding and emerging applications of these materials. In such films, a film-substrate misfit strain enables unprecedented crystal phases and unique properties that are not available in their bulk counterparts. However, the prerequisite growth of strained epitaxial films is fundamentally restricted by misfit relaxation. Beyond usage in advanced integrated devices and as high-quality crystals for basic investigations, epitaxial films bring a plethora of remarkable novel phenomena that stem from couplings between film with underlying substrate.

We demonstrated in this paper that introduction of a small oxygen deficiency concurrently stabilizes epitaxy and increases lattice strain in thin films of archetypal perovskite oxide $SrTiO_3$. By combining experimental and theoretical methods, we found that anisotropic lattice distortions around oxygen vacancies produce elastic dipoles, which interact with the misfit strain in epitaxial films. Consequently, the dipoles are crystallographically aligned, which is energetically favorable and improves epitaxy.

Because anisotropic oxygen-vacancy elastic dipoles are inherent to perovskite-type and many other oxides, we anticipate that the disclosed phenomenon of epitaxial stabilization by oxygen vacancies is relevant for a very broad range of functional oxides.

Published in:

M. Tyunina, L. Rusevich, E. Kotomin, O. Pacherova, A. Dejneka, Epitaxial growth of perovskite oxide films facilitated by oxygen vacancies, *J. Materials Chemistry C* 9 (2021) 1693, doi:10.1039/d0tc0570a.



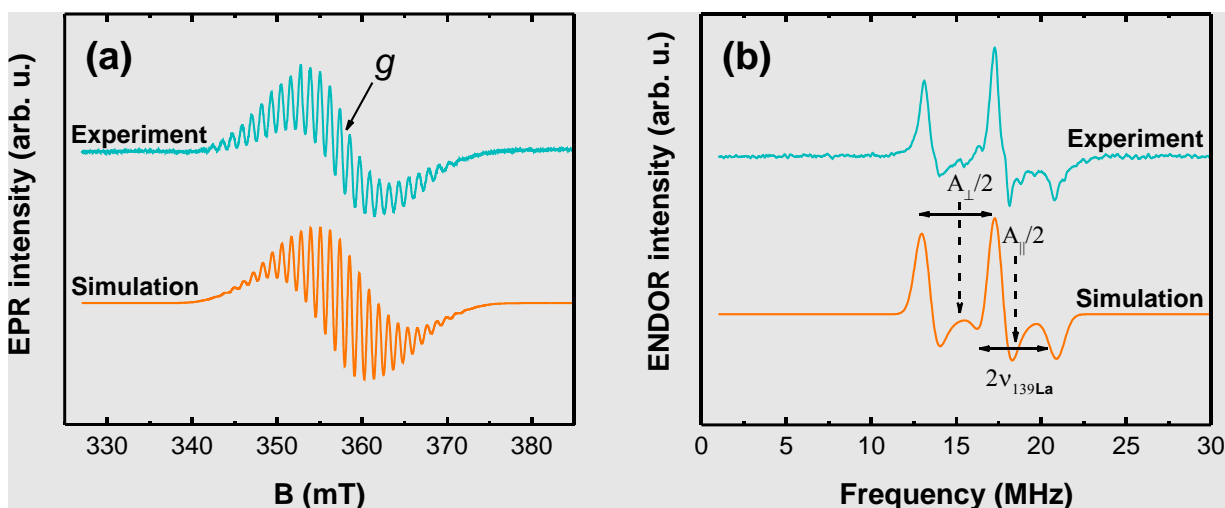
Schematics of ionic positions in (a) regular STO and (b, c) around an oxygen vacancy in STO. In (c), the arrows mark directions of ionic displacements around vacancy compared to regular STO.

Oxidation state and local structure of chromium ions in LaOCl

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Lanthanum oxychloride (LaOCl), which is being considered for a variety of applications including gas sensors, catalysts and solid electrolytes, is one of the most widely investigated compounds from the class of lanthanide oxyhalides. Despite the wide research performed on the host, the incorporation mechanisms of multi-valent impurities in the LaOCl lattice are not fully understood. Therefore, in this study, local structure and oxidation state sensitive X-ray and magnetic resonance spectroscopy techniques were applied to elucidate the mechanism of multivalent chromium ion incorporation in LaOCl.



(a) EPR and (b) ENDOR spectra simulations of LaOCl sample with 0.1 mol% Cr.

It was determined that chromium incorporation in LaOCl occurs predominantly in the 5+ oxidation state producing asymmetric distortions to the crystal structure: a decrease of lattice parameter a and an increase of lattice parameter c . The EPR spectrum of LaOCl:Cr⁵⁺ consists of resonance at $g = 1.964$ with a well-resolved HF structure from interaction with 4 equivalent La nuclei. XRD and EPR data, which are validated by the Cr K-edge XANES simulations, suggest that Cr⁵⁺ incorporation occurs in the voids within the layers of chlorine ions. LaOCl sample annealing in reducing atmosphere affects the oxidation state and the local symmetry of chromium ions. It has been determined that at least two types of axial symmetry Cr³⁺ centers are formed in LaOCl.

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A. Antuzevics, G. Kriekē, H. Ozols, A. Fedotovs, A. Sarakovskis, A. Kuzmin, Oxidation state and local structure of chromium ions in LaOCl, *Materials* **14** (2021) 3539, doi: 10.3390/ma14133539.

Study of high-temperature behaviour of ZnO by ab initio molecular dynamics simulations and X-ray absorption spectroscopy

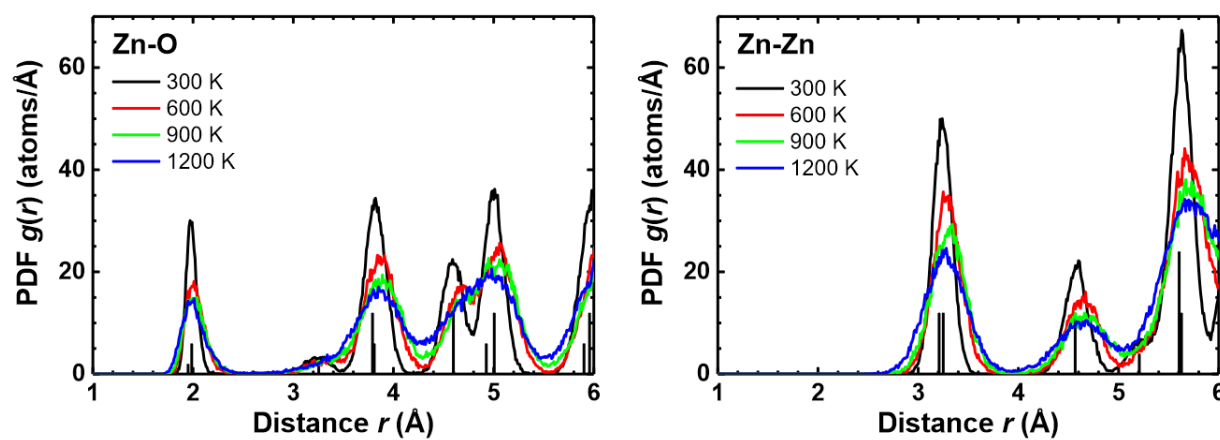
D. Bocharov^a, I. Pudza^a, K. Klementiev^b, M. Krack^c, A. Kuzmin^a

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Wurtzite-type zinc oxide (w-ZnO) is a wide band-gap ($E_g = 3.37$ eV) semiconductor with a pronounced structural anisotropy along the c axis, which affects its lattice dynamics and represents a difficulty for its accurate description using classical models of interatomic interactions. In this study, ab initio molecular dynamics (AIMD) was employed to simulate a bulk w-ZnO phase in the NpT ensemble in the high-temperature range from 300 K to 1200 K. The results of the simulations were validated by comparison with the experimental Zn K-edge extended X-ray absorption fine structure (EXAFS) spectra and known diffraction data.



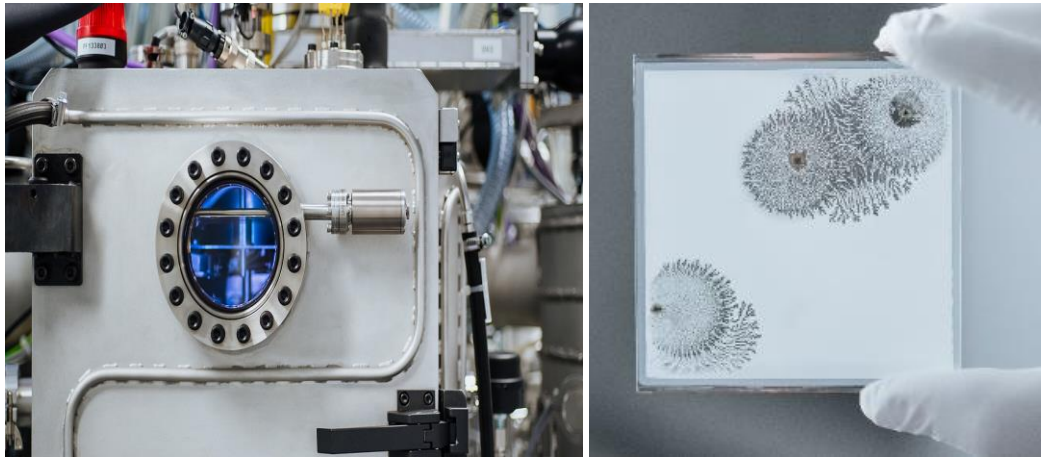
Atomic pair distribution functions (PDFs) around absorbing Zn atom obtained from AIMD calculations in the NpT ensemble at 300, 600, 900 and 1200 K. Vertical lines show crystallographic distances in wurtzite-type ZnO at 300 K.

AIMD NpT simulations reproduced well the thermal expansion of the lattice, and the pronounced anharmonicity of Zn–O bonding was observed above 600 K. The PDFs for Zn–O and Zn–Zn show a significant temperature dependence due to the lattice expansion and the amplitude change of the atomic vibrations. An increase of temperature leads to the broadening of the bond angle distributions, whereas the mean values of the bond angles O–Zn–O and Zn–O–Zn remain almost temperature independent. This fact suggests a weak temperature dependence of the parameter $u(O)$, which determines the distortion of the ZnO_4 tetrahedral, and the piezoelectric coefficients. Our results are in agreement with the previous conclusions based on the neutron diffraction measurements in the temperature range of 20–900 K.

Published in:

D. Bocharov, I. Pudza, K. Klementiev, M. Krack, A. Kuzmin, Study of high-temperature behaviour of ZnO by ab initio molecular dynamics simulations and X-ray absorption spectroscopy, *Materials* **14** (2021) 5206, doi: 10.3390/ma14185206.

Technology and experimental methods.

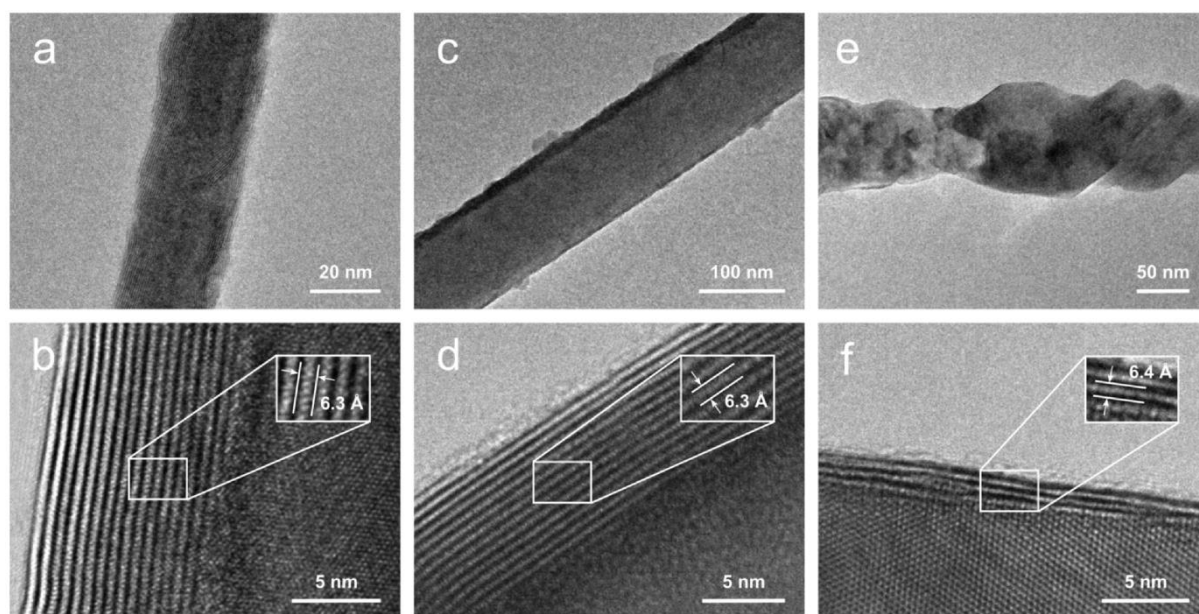


Synthesis and characterization of GaN/ReS₂, ZnS/ReS₂ and ZnO/ReS₂ core/shell nanowire heterostructures

E. Butanovs, A. Kuzmin, S. Piskunov, K. Smits, A. Kalinko, B. Polyakov

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Layered 2D van der Waals (vdW) materials such as graphene and transition metal dichalcogenides have recently gained a great deal of scientific attention due to their unique properties and prospective applications in various fields such as electronics and optoelectronics, sensors and energy. As a direct bandgap semiconductor in both bulk and monolayer forms, ReS₂ stands out for its unique distorted octahedral structure that results in distinctive anisotropic physical properties; however, only a few scalable synthesis methods for few-layer ReS₂ have been proposed thus far. Here, the growth of high-quality few-layer ReS₂ is demonstrated via sulfurization of a pre-deposited rhenium oxide coating on different semiconductor material nanowires (GaN, ZnS, ZnO). As-produced core-shell heterostructures were characterized by X-ray diffraction, scanning and transmission electron microscopy, micro-Raman spectroscopy and X-ray absorption spectroscopy. Experimental characterizations were supported by total energy calculations of the electronic structure of ReS₂ nanosheets and GaN, ZnS, and ZnO substrates. Our results demonstrate the potential of using nanowires as a template for the growth of layered vdW materials to create novel core-shell heterostructures for energy applications involving photocatalytic and electrocatalytic hydrogen evolution.



Transmission electron microscope images at different magnifications for as-grown (a,b) GaN-ReS₂, (c,d) ZnS-ReS₂, and (e,f) ZnO-ReS₂ core-shell nanowires, prepared at 800°C. The insets show the measured atomic interlayer distances between ReS₂ layers.

Published in:

*E. Butanovs, A. Kuzmin, S. Piskunov, K. Smits, A. Kalinko, B. Polyakov, Synthesis and characterization of GaN/ReS₂, ZnS/ReS₂ and ZnO/ReS₂ core/shell nanowire heterostructures, **Appl. Surf. Sci.** 536 (2021) 147841, doi: 10.1016/j.apsusc.2020.147841.*

The role of Ga and Bi doping on the local structure of transparent zinc oxide thin films

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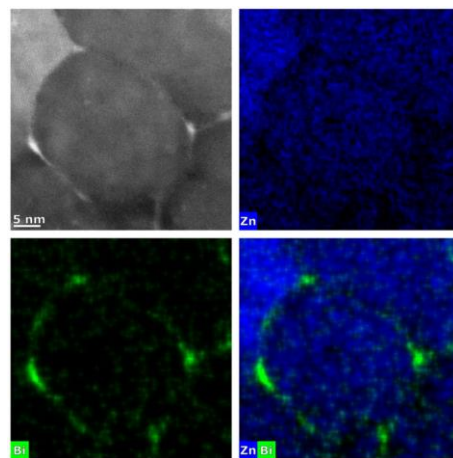
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Transparent undoped ZnO and additionally doped with Ga and Bi thin films were produced by magnetron sputtering and characterized by X-ray absorption spectroscopy (XAS), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), transmission and scanning transmission electron (TEM, STEM) microscopy and Raman spectroscopy. All undoped and doped films crystallise in a ZnO phase with the hexagonal wurtzite crystal structure. The local structure of the thin films was investigated by temperature-dependent XAS at the Zn and Ga K-edges, as well as at the Bi L₃-edge. It was found that the doping of Ga³⁺ and Bi³⁺ ions in the ZnO wurtzite structure produces distinct effects on the thin film microstructure. The substitution of Zn²⁺ ions by smaller Ga³⁺ ions introduces a static disorder to the thin film structure, which is evidenced by an increase in the mean-square relative displacements $\sigma^2(\text{Zn-O})$ and $\sigma^2(\text{Zn-Zn})$. At the same time, large Bi³⁺ ions do not substitute zinc ions, but are likely located in the disordered environment at the ZnO grain boundaries. This conclusion was directly supported by energy-dispersive X-ray spectroscopy combined with TEM and STEM observations as well as by resonant and non-resonant μ -Raman experiments at room temperature, where the ZnO and ZnO:Bi spectra are similar, suggesting a lack of structural disorder in the wurtzite cell. On the other hand, the Raman disorder-activated phonon is pronounced for Ga-doping of the ZnO lattice, confirming the compositional disorder. Both XRD and XPS ruled out Ga₂O₃ phase in Ga-doped ZnO; conversely, Bi₂O₃ and a small amount of Bi-metal phases are clearly discerned by XPS experiments, further suggesting that Bi is not incorporated in the ZnO wurtzite cell, but segregated to grain boundaries.



HAADF-STEM down the [001] zone of the wurzite crystal structure of ZnO and respective Zn and Bi EDX maps for a ZnO:Ga grain of the ZnO:Ga,Bi thin film.

Published in:

F. C. Correia, J. M. Ribeiro, A. Kuzmin, I. Pudza, A. Kalinko, E. Welter, A. Mendes, J. Rodrigues, N. Ben Sedrine, T. Monteiro, M. R. Correia, C. J. Tavares, *The role of Ga and Bi doping on the local structure of transparent zinc oxide thin films*, **J. Alloys Compd.** **870** (2021) 159489, doi: 10.1016/j.jallcom.2021.159489.

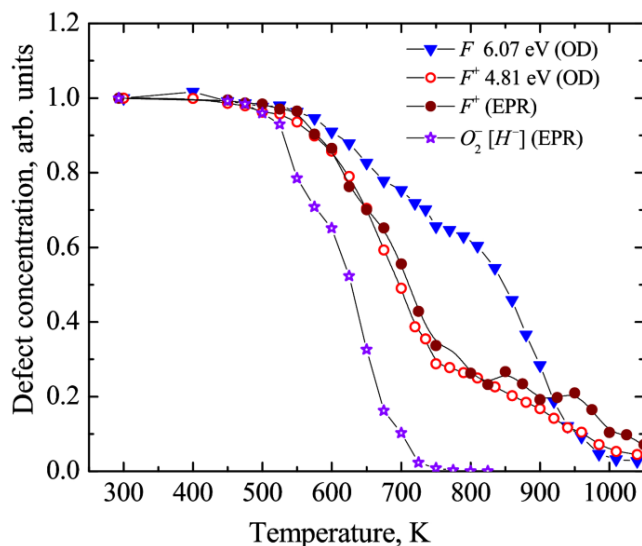
Evidence for the formation of two types of oxygen interstitials in neutron-irradiated α -Al₂O₃ single crystals

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E. Vasil'chenko^{a,b}, A. Popov^{a,b}

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Due to unique optical/mechanical properties and significant resistance to harsh radiation environments, corundum (α -Al₂O₃) is considered as a promising candidate material for windows and diagnostics in forthcoming fusion reactors. However, its properties are affected by radiation-induced (predominantly, by fast neutrons) structural defects. In this study, we analyzed thermal stability and recombination kinetics of primary Frenkel defects in anion sublattice – the *F*-type electronic centers and complementary oxygen interstitials in fast-neutron-irradiated corundum single crystals. Combining precisely measured thermal annealing kinetics for four types of primary radiation defects (neutral and charged Frenkel pairs) and the advanced model of chemical reactions, we have demonstrated for the first time a co-existence of the two types of interstitial defects – neutral O atoms and negatively charged O⁻ ions (with attributed optical absorption bands peaked at energies of 6.5 eV and 5.6 eV, respectively). From detailed analysis of interrelated kinetics of four oxygen-related defects, we extracted their diffusion parameters (interstitials serve as mobile recombination partners) required for the future prediction of secondary defect-induced reactions and, eventually, material radiation tolerance.



Thermal annealing kinetics of the electron-type *F* and *F*⁺ centers as well as O₂⁻ dumbbells (that include H⁻ interstitials). The decay of normalized defect concentrations which were estimated via the absorption band (OD) or EPR signal related to a certain radiation defect.

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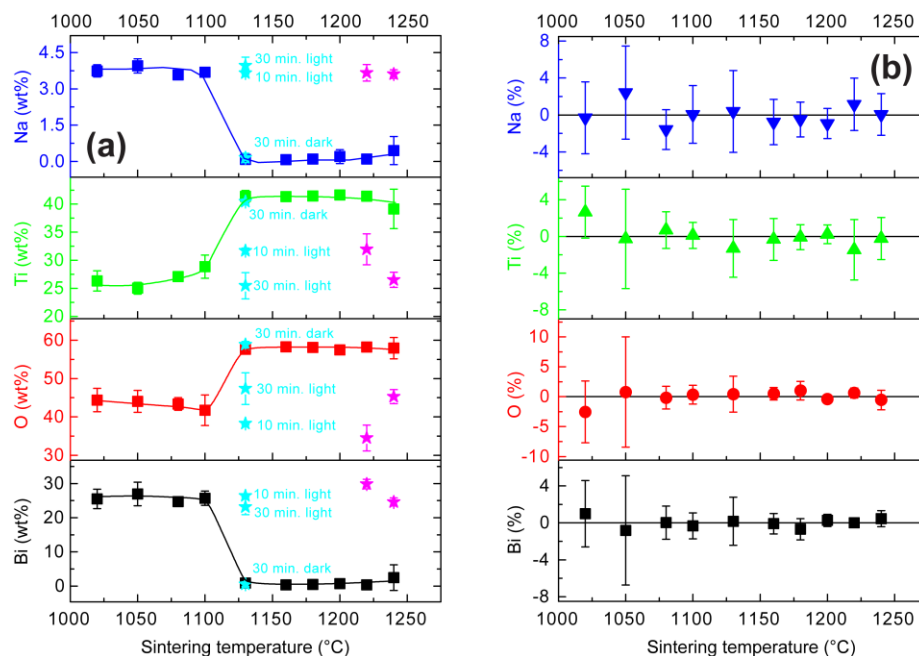
A. Lushchik, V. Kuzovkov, E. Kotomin, G. Prieditis, V. Seeman, E. Shablonin, E. Vasil'chenko, A. Popov, Evidence for the formation of two types of oxygen interstitials in neutron-irradiated α -Al₂O₃ single crystals, *Scientific Reports* **11** (2021) 20909, doi: 10.1038/s41598-021-00336-0.

Influence of sintering temperature on microstructure of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ ceramics

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$\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (NBT)-based ceramics attract interest as one of the most promising lead-free ferroelectrics. Although they are studied a lot regarding modification and improvement of physical properties, there has been very little attention paid to their characterization from the standpoint of processing. In this study, comprehensive analysis of the influence of sintering temperature in range 1020-1240°C on the complete microstructure and chemical content of NBT ceramics produced by solid-state sintering. It is demonstrated how the grain size distribution monotonously broadens with increasing of the average grain size, upon sequential increasing of sintering temperature. Along with high relative density, reaching 98%, two types of pores are observed. Depending on the sintering temperature range, inclusions correspond to the chemical compositions $\text{NaBiTi}_6\text{O}_{14}$ and TiO_2 , as inferred from the local energy-dispersive X-ray analysis.



Concentrations of chemical elements in the inclusions (a), as well as relative deviations from the average concentrations of the chemical elements in the matrix grains (b) of NBT ceramics sintered at different temperatures.

Non-intentional non-stoichiometry is not detected in the matrix grains of the NBT ceramics, even if sintered at high temperatures. It is inferred that, instead of changing the composition of the matrix grains, Na and Bi volatilization rather influences the porosity and inhomogeneity of NBT.

Published in:

*M. Dunce, E. Birks, M. Antonova, L. Bikse, S. Dutkevica, O. Freimanis, M. Livins, L. Eglite, K. Smits, Influence of sintering temperature on microstructure of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ ceramics, *J. Alloy. Compd.* **884** (2021) 160955, doi: 10.1016/j.jallcom.2021.160955.*

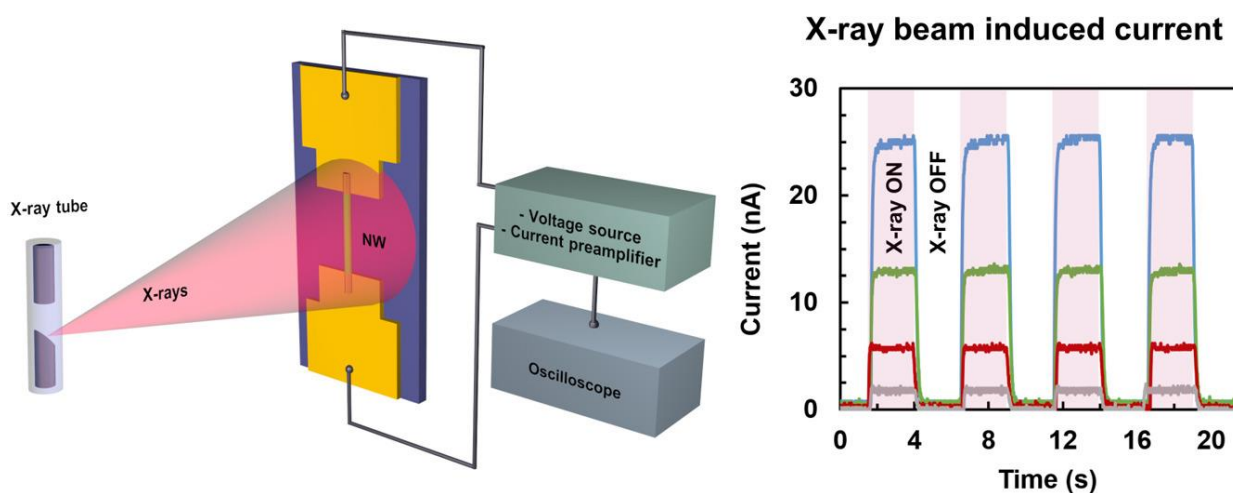
Nanoscale X-ray detectors based on individual CdS, SnO₂ and ZnO nanowires

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The development of nanoscale X-ray sensors is of crucial importance to achieve higher spatial resolution in many X-ray-based techniques playing a key role in materials science, healthcare, and security. Here, we demonstrate X-ray detection using individual CdS, SnO₂, and ZnO nanowires (NWs). The NWs were produced via vapor–liquid–solid technique and characterized using X-ray diffraction, scanning, and transmission electron microscopy.

Electrical measurements were performed under ambient conditions while exposing two-terminal NW-based devices to X-rays generated by a conventional tungsten anode X-ray tube. Fast and stable nanoampere-range X-ray beam induced current (XBIC) in response to X-ray illumination was observed. The high XBIC measured in the NW devices could be attributed to the efficient transport and collection of generated charge carriers due to the single-crystalline nature of NWs and the short NW length. Such fast-response and high-sensitivity nanoscale X-ray detectors can find applications in sub-micron resolution imaging and nanofocused beam shape measurements.



Schematic of the experimental setup (left panel). A single nanowire (NW) device on a Si/SiO₂ substrate was illuminated with X-rays, generated by a tungsten anode X-ray tube. X-ray beam induced current (right panel) was measured by connecting the device to a low-noise current preamplifier and oscilloscope.

Published in:

E. Butanovs, A. Zolotarjovs, A. Kuzmin, B. Polyakov, Nanoscale X-ray detectors based on individual CdS, SnO₂ and ZnO nanowires, Nucl. Instrum. Methods Phys. Res. A 1014 (2021) 165736, doi: 10.1016/j.nima.2021.165736.

Nonlinear absorption and refraction of picosecond and femtosecond pulses in HgTe quantum dot films

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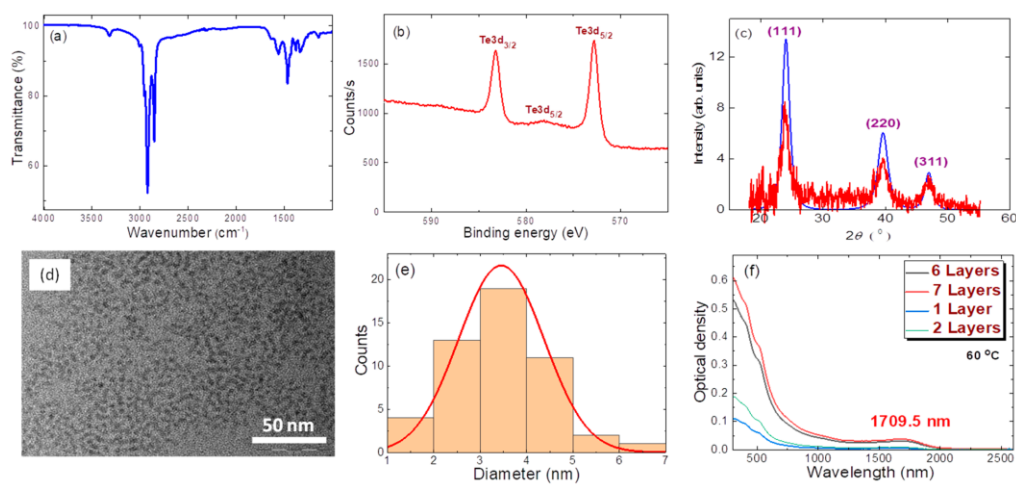
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The saturated intensities, saturable absorption, and nonlinear refraction were measured in 70-nm thick films containing 4 nm HgTe quantum dots. Strong nonlinear refraction and saturable absorption were demonstrated in the thin films using tunable picosecond and femtosecond pulses. Studies were carried out using tunable laser pulses in the range of 400–1100 nm. A significant variation of the nonlinear refraction along this spectral range was demonstrated. The maximal values of the nonlinear absorption coefficients and nonlinear refractive indices determined within the studied wavelength range were $-2.4 \times 10^{-5} \text{ cm}^2 \text{ W}^{-1}$ (in the case of 28 ps, 700 nm probe pulses) and $-3 \times 10^{-9} \text{ cm}^2 \text{ W}^{-1}$ (in the case of 28 ps, 400 nm probe pulses), respectively. Our studies show that HgTe quantum dots can be used in different fields e.g., as efficient emitters of high-order harmonics of ultrashort laser pulses or as laser mode-lockers.



HgTe quantum dots: (a) FTIR spectra in the range of 5000–800 cm^{-1} . (b) High-resolution XPS spectrum. (c) X-ray diffraction image. Blue curve: calculation. Red curve: experiment. (d) TEM image. (e) Histogram of particles distribution. (f) Vis-IR absorption spectra of thin films.

Published in:

A. Bundulis, I. Shuklov, V. Kim, A. Mardini, J. Grube, J. Alnis, A. Lizunova, V. Razumov, R. Ganeev, *Nonlinear absorption and refraction of picosecond and femtosecond pulses in HgTe quantum dot films*, **Nanomaterials** **11** (2021) 3351, doi: 10.3390/nano11123351.

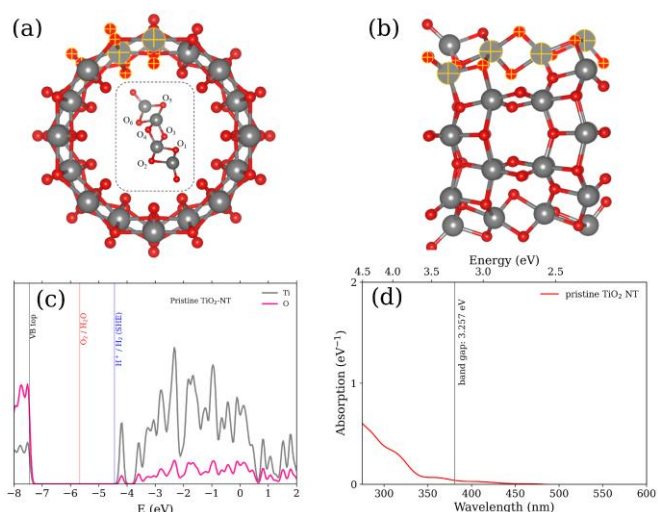
Time-dependent density functional theory calculations of N- and S-doped TiO₂ nanotube for water-splitting applications

Y.-P. Lin^a, I. Isakoviča^a, A. Gopejenko^a, A. Ivanova^a, A. Začinskis^a, R. Eglitis^a, P. D'yachkov^b, S. Piskunov^a

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Use of photodriven semiconductor-based catalyst is a promising route for energy production from sunlight. One of the main directions in this respect is utilization of the solar power for producing hydrogen fuel through the photocatalytic water-splitting reaction. Among all photocatalytic materials, titania (TiO₂) has been widely investigated in the past. On the basis of time-dependent density functional theory (TD-DFT) we performed first-principle calculations to predict optical properties and transition states of pristine, N- and S-doped, and N+S-codoped anatase TiO₂ nanotubes of 1 nm-diameter. The host O atoms of the pristine TiO₂ nanotube (NT) were substituted by N and S atoms to evaluate the influence of dopants on the photocatalytic properties of hollow titania nanostructures. The charge transition mechanism promoted by dopants positioned in the nanotube wall clearly demonstrates the constructive and destructive contributions to photoabsorption by means of calculated transition contribution maps. Based on the results of our calculations, we predict an increased visible-light-driven photoresponse in N- and S-doped and the N+S-codoped TiO₂ nanotubes, enhancing the efficiency of hydrogen production in water-splitting applications.



Schematic illustration of the pristine (8,0) anatase (101) TiO₂ NT with the diameter of 0.933 nm: (a) front view of the NT, and (b) side view of the NT. Ti atoms are shown as gray balls, oxygens are shown as red balls. The inset in (a) shows the unit cell of the TiO₂ NT repeated 8 times by rototranslational symmetry. The numbered O atoms denote the doping sites. (c) The projected density of states (PDOS) of pristine TiO₂ NT as calculated by means of GLLB-SC exchange–correlation functional within DFT. Vertical black line crossing the DOS plot corresponds to VBM of the pristine TiO₂ NT, while red and blue lines correspond to O₂/H₂O and H⁺/H₂ redox potentials with respect to the vacuum level, respectively. (d) is the calculated optical absorption spectrum of the pristine TiO₂ NT. Vertical black line crossing the spectrum corresponds to the band gap width of the pristine TiO₂ NT.

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Y.-P. Lin, I. Isakoviča, A. Gopejenko, A. Ivanova, A. Začinskis, R. Eglitis, P. D'yachkov, S. Piskunov, Time-dependent density functional theory calculations of N- and S-doped TiO₂ nanotube for water-splitting applications, *Nanomaterials* **11** (2021) 2900, doi: 10.3390/nano11112900.

Positron annihilation lifetime spectroscopy insight on free volume conversion of nanostructured MgAl₂O₄ ceramics

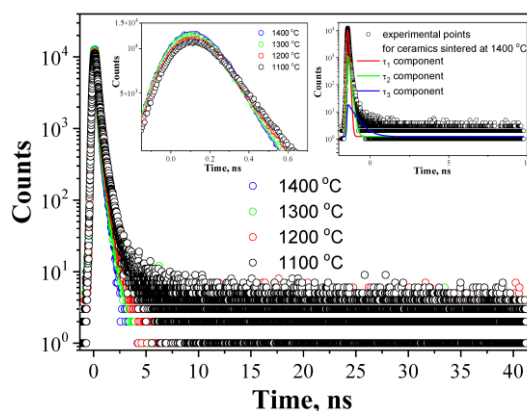
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Positron annihilation lifetime spectroscopy (PALS) technique is considered as one of the promising alternative methods to analyze free volume and defects in functional and other materials. Herein we demonstrate the specifics of using the positron annihilation lifetime spectroscopy (PALS) method for the study of free volume changes in functional ceramic materials. Choosing technological modification of nanostructured MgAl₂O₄ spinel as an example, we show that for ceramics with well-developed porosity positron annihilation is revealed through two channels: positron trapping channel and ortho-positronium decay. Positron trapping in free-volume defects is described by the second component of spectra and ortho-positronium decay process by single or multiple components, depending on how well porosity is developed and on the experimental configuration. When using proposed positron annihilation lifetime spectroscopy approaches, three components are the most suitable fit in the case of MgAl₂O₄ ceramics. In the analysis of the second component, it is shown that technological modification (increasing sintering temperature) leads to volume shrinking and decreases the number of defect-related voids. This process is also accompanied by the decrease of the size of nanopores (described by the third component), while the overall number of nanopores is not affected. The approach to the analysis of positron annihilation lifetime spectra presented here can be applied to a wide range of functional nanomaterials with pronounced porosity.



PALS spectra for MgAl₂O₄ ceramics sintered at 1100-1400 °C for 2 h with three components decomposition curves for ceramics sintered at 1400 °C.

Published in:

H. Klym, I. Karbovnyk, S. Piskunov, A. Popov, Positron annihilation lifetime spectroscopy insight on free volume conversion of nanostructured MgAl₂O₄ ceramics, *Nanomaterials* **11** (2021) 3373, doi: 10.3390/nano11123373.

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



The luminescent properties of SrAl₂O₄: Eu, Dy, B doped phosphate glasses for low-temperature applications

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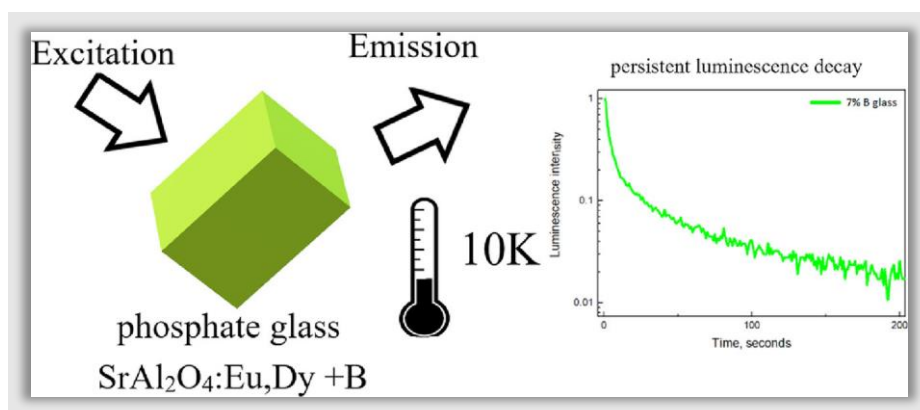
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SrAl₂O₄: Eu, Dy, B particles were added in a phosphate glass (90NaPO₃-10NaF (in mol%)) using the direct doping method. For the first time, the composition of the particles before and after embedding them in the glass was analysed using EPMA analysis. Boron was found to be incorporated in already distorted surroundings creating new trapping centers in the particles which are thought to be favourable for the tunnelling process and so for the afterglow at 10K. Despite the partial decomposition of the particles, the glass exhibit afterglow at low temperature confirming to be promising materials for low-temperature applications.



In summary, phosphate glasses containing SrAl₂O₄: Eu, Dy, B were successfully prepared with persistent luminescence at low temperature by adding the B containing PL particles in the glass melt. From the EPMA analysis of the particles alone, B tends to incorporate in already distorted crystal lattice surroundings in the proximity of those Sr lattice sites, that have been replaced by Dy. The addition of B presumably creates different lattice distortions, that can lead to electron trapping. The afterglow decay of the glasses was considerably lower compared to that of the particles alone due to the decomposition of the particles occurring during the glass preparation. However, due to B in the particles, the glass-based materials exhibit afterglow at low temperatures creating possible sensing and biomedical applications.

Published in:

V. Vitola, V. Lahti, I. Bite, A. Spustaka, D. Millers, M. Lastusaari, L. Petit, K. Smits, Low temperature afterglow from SrAl₂O₄: Eu, Dy, B containing glass, *Scripta Materialia* **190** (2021) 86-90, doi: 10.1016/j.scriptamat.2020.08.023.

Triboelectrification of nanocomposites using identical polymer matrixes with different concentrations of nanoparticle fillers

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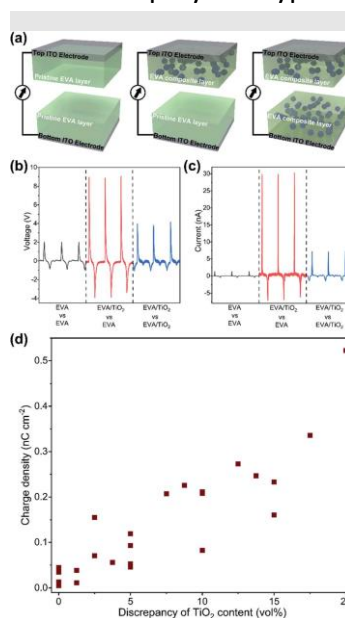
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Triboelectrification in polymer-based nanocomposites using identical polymer matrixes containing different concentrations of nanoparticles (NPs) was studied. The triboelectric surface charge density on polymer layers increased as the difference in nanoparticle filler concentration between the two triboelectric layers escalated, even though the polymer matrix was the same in both layers. This effect was observed in tests of various polymer types and filler NPs. Mechanical experiments and finite element simulations confirmed that polymeric triboelectrification is related to the surface viscoelastic deformation that occurs during mechanical contact and separation and does not depend on electronic or chemical properties but rather on physicochemical and mechanical properties. The triboelectrification of polymeric materials is inextricably linked to the mass transfer mechanism that is consistent with previous research. Our findings will assist in developing efficient triboelectric devices or protective structures that rely on polymer materials.



Published in:

L. Lapčinskis, A. Linarts, K. Mālnieks, H. Kim, K. Rubenis, K. Pudzs, K. Smits, A. Kovaļovs, A. Tamm, C.K. Jeong, A. Šutka, Triboelectrification of nanocomposites using identical polymer matrixes with different concentrations of nanoparticle fillers, *Journal of Materials Chemistry A* 9 (2021) 8984-8990, doi: 10.1039/D0TA12441A.

Time-resolved FDTD and experimental FTIR study of gold micropatch arrays for wavelength-selective mid-infrared optical coupling

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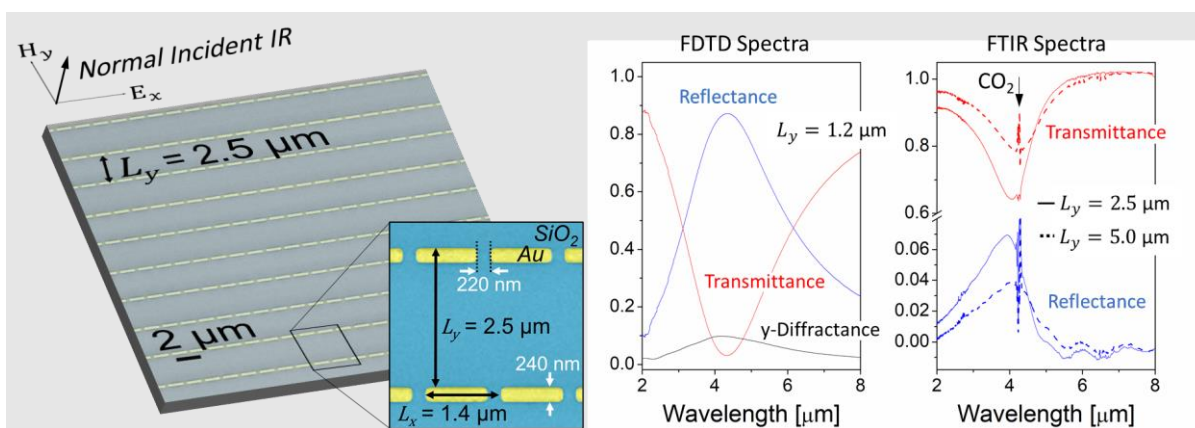
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Photonic metasurface arrays show great promise for applications in photodetection and infrared molecular sensing (e.g. CO₂, alcohol). The optical response can be precisely controlled by fine adjustments of the metasurface geometry.

In this paper, infrared radiation reflection and transmission of a single layer of gold micropatch two-dimensional arrays, of patch length $\sim 1.0 \mu\text{m}$ and width $\sim 0.2 \mu\text{m}$, have been carefully studied by a finite-difference time-domain (FDTD) method, and Fourier-transform infrared spectroscopy (FTIR).

Through the precision design of the micropatch array structure geometry, we achieve a significantly enhanced reflectance (85%), substantial diffraction (10%), and a much-reduced transmittance (5%) for an array of only 15% surface metal coverage. This results in an efficient far-field optical coupling with promising practical implications for efficient mid-infrared photodetectors.

Most importantly we find that the propagating electromagnetic fields are transiently concentrated around the gold micropatch array in a time duration of tens of ns, providing us with a novel efficient near-field optical coupling.



Gold nanoantenna array metasurface with corresponding FDTD and FTIR spectra.

Published in:

Y. Fu, T. Yager, G. Chikvaidze, S. Iyer, Q. Wang, Time-resolved FDTD and experimental FTIR study of gold micropatch arrays for wavelength-selective mid-infrared optical coupling, *Sensors* **21** (2021) 5203, doi: 10.3390/s21155203.

Changes in surface free energy and surface conductivity of carbon nanotube/polyimide nanocomposite films induced by UV irradiation

B. Zhang^a, M. Clausi^b, B. Heck^c, S. Laurenzi^b, M. G. Santonicola^b, J. Kleperis^d, A. Antuzevičs^d, G. Reiter^c, A. N. Aleshin^e, A. S. Lobach^e

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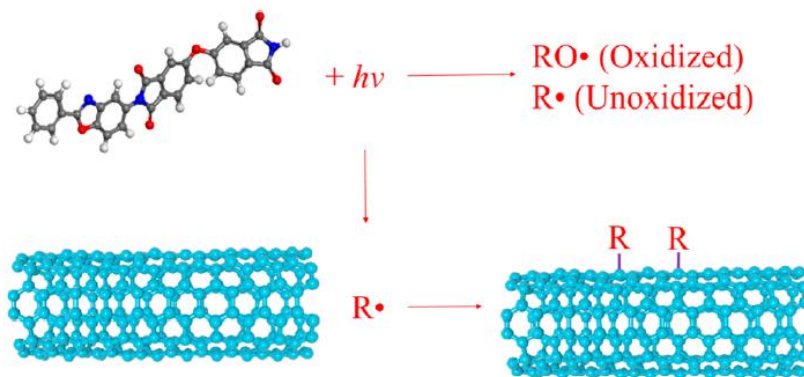
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Changes in surface energy and electrical conductivity of polyimide (PI)-based nanocomposite films filled with carbon nanotubes (CNTs) induced by UV exposure are gaining considerable interest in microelectronic, aeronautical, and aerospace applications. However, the underlying mechanism of PI photochemistry and oxidation reactions induced by UV irradiation upon the surface in the presence of CNTs is still not clear. In this work, the interplay between CNTs and PIs under UV exposure in the surface properties of CNT/PI nanocomposite films was probed.



Proposed model of radical changes undergoing photochemical reaction and oxidization in the presence of CNTs.

The consequences of changes in the chemical nature of the surface of PI and CNT/PI nanocomposite films after UV irradiation in terms of the surface energy and surface conductivity of CNT/PI nanocomposite films have been investigated. The highest conductivity was observed in UV-C irradiated CNT/PI nanocomposite films. It was attributed to the hopping of unpaired electrons from aromatic ring sites to aromatic ring sites and the high intrinsic conductivity of CNTs.

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B. Zhang, M. Clausi, B. Heck, S. Laurenzi, M.G. Santonicola, J. Kleperis, A. Antuzevičs, G. Reiter, A.N. Aleshin, A.S. Lobach, Changes in Surface Free Energy and Surface Conductivity of Carbon Nanotube/Polyimide Nanocomposite Films Induced by UV Irradiation, *ACS Appl. Mater. Interfaces*. **13** (2021) 24218-24227, doi: 10.1021/acami.1c02654.

All-organic fast intersystem crossing assisted exciplexes exhibiting sub-microsecond thermally activated delayed fluorescence

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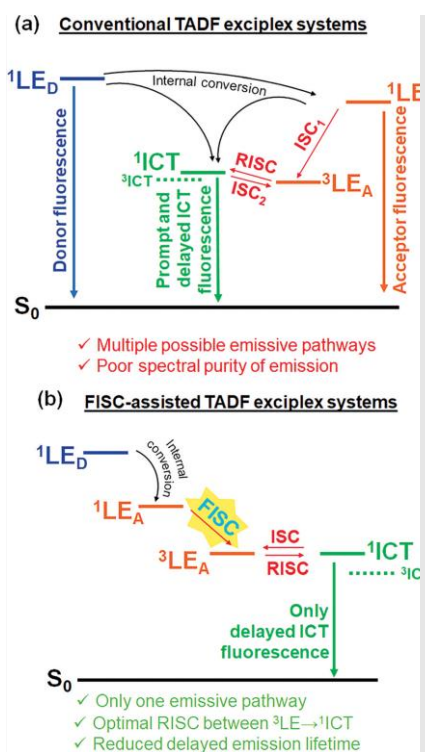
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A novel strategy is presented towards acquisition of exciplex systems exhibiting thermally activated delayed fluorescence (TADF) with a high reverse intersystem crossing (RISC) rate (exceeding 10^7 s^{-1}). This approach involves constructing exciplex donor–acceptor molecular pairs, where the acceptor molecule possesses the ability to undergo fast and efficient intersystem crossing (ISC). With the use of 6-cyano-9-phenylpurine (PCP) acceptor and carbazole-based donor molecules, exciplexes were obtained, where the excitation is contained on PCP and undergoes fast ISC to form a local excited triplet state ($^3\text{LE}_A$). The controlled excitation transfer to the $^3\text{LE}_A$ level provides an optimal reverse intersystem crossing pathway, enabling TADF with a sub-microsecond emission lifetime. The side-effect of such an emissive mechanism is an unusual thermal photoluminescence quenching, caused by the limited PCP triplet state stability under room temperature conditions. PCP-carbazole dyads were obtained, which, in neat solid films, form intermolecular TADF-active exciplexes between donor and acceptor fragments of the neighbouring molecules. These compounds show balanced bipolar charge transport ability and were used as emissive layer host materials. The obtained organic light emitting diode (OLED) with an exciplex-forming host and a TADF emitter showed an external quantum efficiency exceeding 10% and low efficiency roll-off.



Schematic representation of the emission processes for conventional (a) and FISC-assisted TADF exciplex systems (b).

Published in:

K. Traskovskis, A. Sebris, I. Novosjolova, M. Turks, M. Guzauskas, D. Volyniuk, O. Bezikonny, J. V. Grazulevicius, A. Mishnev, R. Grzibovskis, Aivars Vembris, All-organic fast intersystem crossing assisted exciplexes exhibiting sub-microsecond thermally activated delayed fluorescence, *J. Mater. Chem. C* **9** (2021) 4532, doi: 10.1039/d0tc05099g.

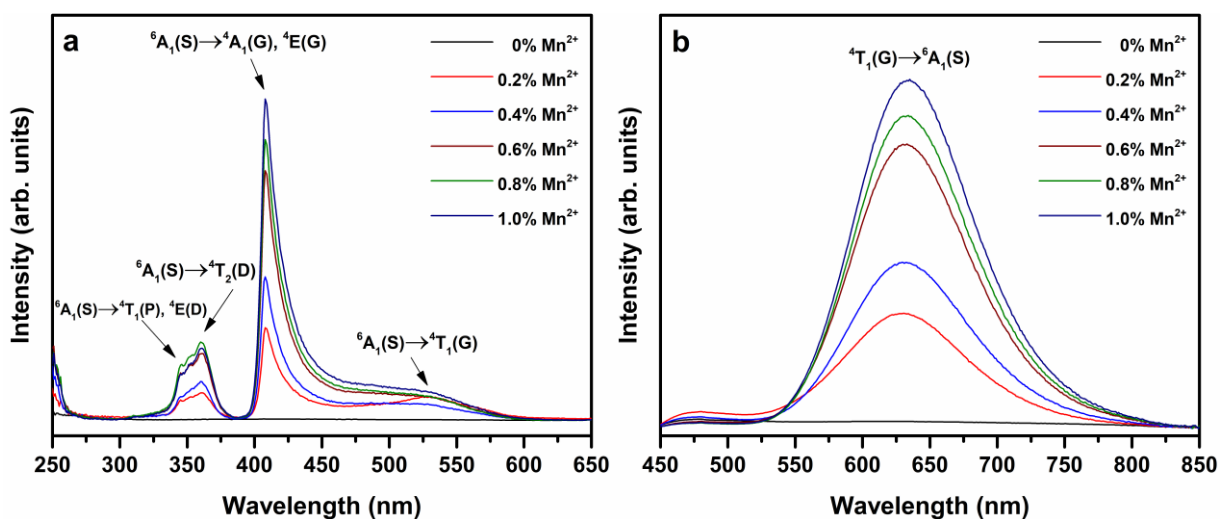
Synthesis and luminescent properties of Mn-doped alpha tricalcium phosphate

L. Sinusaite^a, A. Antuzevics^b, A. I. Popov^b, U. Rogulis^b, M. Misevicius^a, A. Katelnikovas^a,
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Synthetic calcium phosphates (CPs) are widely used for regenerative medicine purposes due to their biological properties and compositional similarity to natural human bone. One of the most popular and frequently used CP is tricalcium phosphate (TCP, $\text{Ca}_3(\text{PO}_4)_2$). It has two polymorphs, which can be stabilized at room temperature, and both of them are used for biomedical applications as injectable bone fillers or ceramic substitutes. The main aim of this study was to investigate the feasibility of the synthesis of Mn-doped α -TCP and to study its structural and luminescent properties



Excitation ($\lambda_{em} = 670$ nm) and emission ($\lambda_{ex} = 408$ nm) spectra of Mn²⁺-doped α -TCP.

A series of Mn²⁺-doped α -TCP powders with a doping level ranging from 0.2 to 1 mol% were successfully synthesized by co-precipitation method followed by high-temperature annealing and thermal quenching. The optical properties of the synthesized specimens were investigated in terms of PL. It was demonstrated that Mn-containing powders under excitation at 408 nm revealed a broadband emission in the range from 525 to 825 nm with a maximum centered at around 630 nm. Emission intensity was found to be dependent on the concentration of Mn ions and increased as Mn content increased. On the contrary, PL lifetimes showed a gradual decrease with an increase of Mn content. Temperature-dependent measurements of PL exhibited a gradual and significant increase of emission intensity at lower temperatures.

Published in:

L. Sinusaite, A. Antuzevics, A.I. Popov, U. Rogulis, M. Misevicius, A. Katelnikovas, A. Kareiva, A. Zarkov, Synthesis and luminescent properties of Mn-doped alpha-tricalcium phosphate, *Ceram. Int.* **47** (2021) 5335–5340, doi: 10.1016/j.ceramint.2020.10.114.

Radiation-induced stable radicals in calcium phosphates: results of multifrequency EPR, EDNMR, ESEEM, and ENDOR studies

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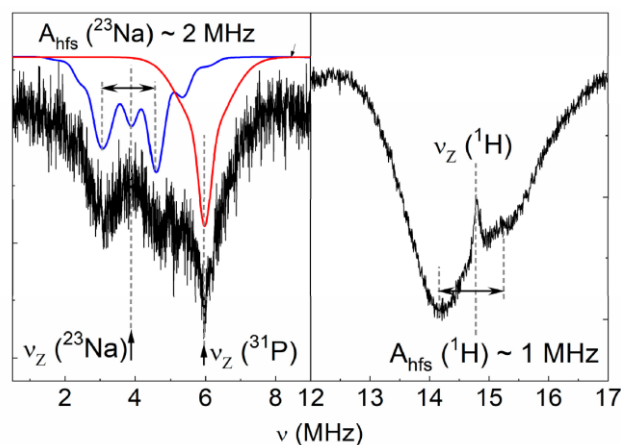
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Currently, calcium phosphate (CP) materials are widely used in orthopedics and dentistry owing to their high biocompatibility and physico-chemical similarity with human hard tissue. This article presents the results of a study of radiation-induced defects in various synthetic CP powder materials (hydroxyapatite—HA and octacalcium phosphate—OCP) by electron paramagnetic resonance (EPR) spectroscopy at the X, Q, and W-bands.



X-band ENDOR spectra detected at $T = 100\text{K}$ of the OCP sample after X-ray irradiation.

It is shown that in addition to the classical EPR techniques, other experimental approaches such as ELDOR-detected NMR (EDNMR), electron spin echo envelope modulation (ESEEM), and electronuclear double resonance (ENDOR) can be used to analyze the electron-nuclear interactions of CP powders. We demonstrated that the value and angular dependence of the quadrupole interaction for ^{14}N nuclei of nitrate radical can be determined by the EDNMR method at room temperature. The ESEEM technique has allowed for rapid analysis of the nuclear environment and estimation of the structural positions of radiation-induced centers in various crystal matrices. ENDOR spectra can provide information about the distribution of the nitrate radicals in the OCP structure.

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Improvement of vacuum characteristics of cryostats for HPGe gamma-radiation detectors

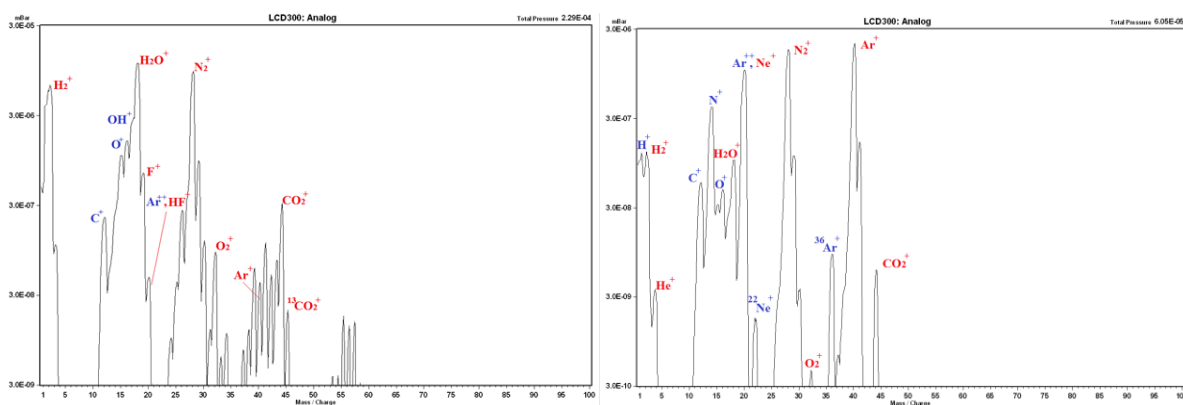
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High-purity germanium (HPGe) crystals are widely used in energy-dispersive (spectrometric) gamma-ray detectors. These devices must be operated at cryogenic temperatures under vacuum conditions. High vacuum (low pressure of the residual gases) is desirable both for thermal insulation and in order to avoid condensation on the surfaces of detector crystal, which increases leakage currents and detector noise, and decreases its energy-resolution. Keeping high vacuum in cryostat for a long time is a formidable task, in particular in thermo-cycled cryostats, where the temperature of the detector crystal is repeatedly cycled between room temperature and cryogenic temperatures.

The present study explores the usability of a recently marketed new chemical getter ("Combogetter"), which bounds the residual gas molecules by chemical reactions. The effect of this type of getter on the composition and time-evolution of residual gases in the detector vacuum chamber was studied. The analysis was performed by quadrupole mass-spectrometer with electron ionization source (RGA analyzer Dycor LC-D (mass range 1–300 amu)).



Residual gas pressure in HPGe detector cryostat with Combogetter immediately after the evacuation (the left panel) and after 96 hours (the right panel). Ordinate scales are logarithmic and equal in both panels. An efficient adsorption of water, O₂, CO₂ and organic contaminants (mass numbers 53...58) is evident. In contrast, the pressure of inert gases and nitrogen keeps increasing.

The measurements confirmed that the (disposable) chemical getter is efficient in maintaining passive (non-pumped) vacuum in HPGe detectors for extended time periods at room temperature. The chemical getter is not useful against accumulation of inert gases, while it is highly efficient in removing water and organic contaminants.

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X-ray diffraction and multifrequency EPR study of radiation-induced room temperature stable radicals in octacalcium phosphate

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V. S. Komlev^b

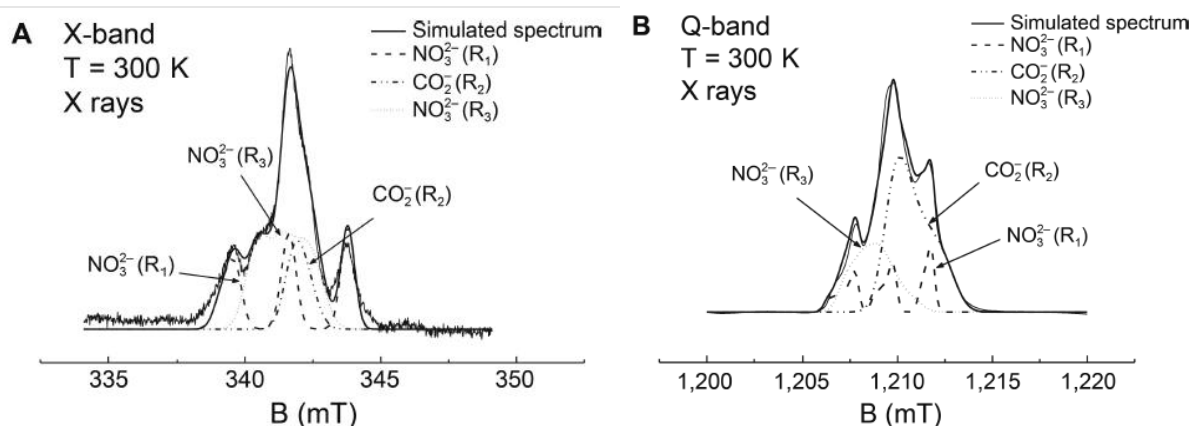
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Octacalcium phosphate (OCP $\text{Ca}_8\text{H}_2(\text{PO}_4)_6 \cdot 5\text{H}_2\text{O}$) has attracted increasing attention over the last decade as a transient intermediate to the biogenic apatite for bone engineering and in studies involving the processes of pathological calcification. In this work, OCP powders obtained by hydrolysis of dicalcium phosphate dehydrate were subjected to X- and γ -ray irradiation and studied by means of stationary and pulsed electron paramagnetic resonance at 9, 36 and 94 GHz microwave frequencies.



Field-swept ESE spectra of OCP sample after X-ray irradiation at X- and Q-bands

Decomposition of the EPR spectra obtained at three frequencies (X-, Q-, W-bands) can be explained by the presence of isotropic (H^0 , CO_3^{3-}) paramagnetic centers and centers of axial symmetry (R_1 – R_3), which we ascribe to carbonate and nitrogen-containing species. ESEEM and ENDOR spectra at X-band reveal the interaction of R_1 – R_3 radicals with ^1H , ^{23}Na and ^{31}P nuclei. Interaction parameters with the ^{23}Na nuclei have been determined. Analysis of EPR, ESSEM and ENDOR results suggests that the obtained paramagnetic species are localized, not in the apatite, but in the hydrated layers of OCP.

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**Publications with the
authorship of ISSP UL in
Web of Science and Scopus
Databases**

- [1] M. Dunce, E. Birks, M. Antonova, L. Bikse, S. Dutkevica, O. Freimanis, M. Livins, L. Eglite, K. Smits, A. Sternberg, Influence of sintering temperature on microstructure of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ ceramics, *Journal of Alloys and Compounds* 884 (2021) 160955.
[DOI: 10.1016/j.jallcom.2021.160955](https://doi.org/10.1016/j.jallcom.2021.160955)
- [2] Y. Mastrikov, N. Chuklina, M. Sokolov, A. Popov, D. Gryaznov, E. Kotomin, J. Maier, Small radius electron and hole polarons in PbX_2 (X= F, Cl, Br) crystals: A computational study, *Journal of Materials Chemistry C* 9 (2021) 16536–16544.
[DOI: 10.1039/d1tc01731d](https://doi.org/10.1039/d1tc01731d)
- [3] Y. Zhdachevskyy, Y. Hizhnyi, S. Nedilko, I. Kudryavtseva, V. Pankratov, V. Stasiv, L. Vasylechko, D. Sugak, A. Lushchik, M. Berkowski, A. Suchocki, N. Klyui, Band Gap Engineering and Trap Depths of Intrinsic Point Defects in RAIO_3 (R = Y, La, Gd, Yb, Lu) Perovskites, *Journal of Physical Chemistry C* 125 (2021) 26698–26710.
[DOI: 10.1021/acs.jpcc.1c06573](https://doi.org/10.1021/acs.jpcc.1c06573)
- [4] H. Klym, I. Karbovnyk, S. Piskunov, A. Popov, Positron annihilation lifetime spectroscopy insight on free volume conversion of nanostructured MgAl_2O_4 ceramics, *Nanomaterials* 11 (2021) 3373.
[DOI: 10.3390/nano11123373](https://doi.org/10.3390/nano11123373)
- [5] D. Sergejev, N. Zhanturina, A. Aizharikov, A. Popov, Influence of “productive” impurities (Cd, Na, O) on the properties of the $\text{Cu}_2\text{ZnSnS}_4$ absorber of model solar cells, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 13–23.
[DOI: 10.2478/lpts-2021-0042](https://doi.org/10.2478/lpts-2021-0042)
- [6] V. Karitans, M. Ozolinsh, A. Lapins, S. Fomins, The effect of the range of a modulating phase mask on the retrieval of a complex object from intensity measurements, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 3–12.
[DOI: 10.2478/lpts-2021-0041](https://doi.org/10.2478/lpts-2021-0041)
- [7] A. Knoks, J. Kleperis, G. Bajars, L. Grinberga, O. Bogdanova, WO_3 as additive for efficient photocatalyst binary system TiO_2/WO_3 , *Latvian Journal of Physics and Technical Sciences* 58 (2021) 24–34.
[DOI: 10.2478/lpts-2021-0043](https://doi.org/10.2478/lpts-2021-0043)
- [8] B. Straumal, E. Rabkin, G. Lopez, A. Korneva, A. Kuzmin, A. Gornakova, A. Straumal, B. Baretzky, Grain boundary wetting phenomena in high entropy alloys containing nitrides, carbides, borides, silicides, and hydrogen: A review, *Crystals* 11 (2021) 1540.
[DOI: 10.3390/cryst11121540](https://doi.org/10.3390/cryst11121540)
- [9] H. Klym, I. Karbovnyk, A. Luchechko, Y. Kostiv, V. Pankratova, A. Popov, Evolution of free volumes in polycrystalline BaGa_2O_4 ceramics doped with Eu^{3+} ions, *Crystals* 11 (2021) 1515.
[DOI: 10.3390/cryst11121515](https://doi.org/10.3390/cryst11121515)
- [10] B. Straumal, A. Korneva, G. Lopez, A. Kuzmin, E. Rabkin, G. Gerstein, A. Straumal, A. Gornakova, Grain boundary wetting by a second solid phase in the high entropy alloys: A review, *Materials* 14 (2021) 7506.
[DOI: 10.3390/ma14247506](https://doi.org/10.3390/ma14247506)
- [11] L. Rusevich, M. Tyunina, E. Kotomin, N. Nepomniashchaia, A. Dejneka, The electronic properties of $\text{SrTiO}_{3-\delta}$ with oxygen vacancies or substitutions, *Scientific Reports* 11 (2021) 23341.

[DOI: 10.1038/s41598-021-02751-9](https://doi.org/10.1038/s41598-021-02751-9)

- [12] A. Bundulis, I. Shuklov, V. Kim, A. Mardini, J. Grube, J. Alnis, A. Lizunova, V. Razumov, R. Ganeev, Nonlinear absorption and refraction of picosecond and femtosecond pulses in HgTe quantum dot films, *Nanomaterials* 11 (2021) 3351.
[DOI: 10.3390/nano11123351](https://doi.org/10.3390/nano11123351)
- [13] A. Usseinov, Z. Koishybayeva, A. Platonenko, V. Pankratov, Y. Suchikova, A. Akilbekov, M. Zdorovets, J. Purans, A. Popov, Vacancy defects in Ga₂O₃: First-principles calculations of electronic structure, *Materials* 14 (2021) 7384.
[DOI: 10.3390/ma14237384](https://doi.org/10.3390/ma14237384)
- [14] H. Van Der Meiden, S. Almaviva, J. Butikova, V. Dwivedi, P. Gasior, W. Gromelski, A. Hakola, X. Jiang, I. J. J. J. Karhunen, M. Kubkowska, M. Laan, G. Maddaluno, A. Marín-Roldán, P. Paris, K. Piip, M. Písarčík, G. Sergienko, M. Veis, P. Veis, S. Brezinsek, Monitoring of tritium and impurities in the first wall of fusion devices using a libs based diagnostic, *Nuclear Fusion* 61 (2021) 125001.
[DOI: 10.1088/1741-4326/ac31d6](https://doi.org/10.1088/1741-4326/ac31d6)
- [15] P. Rodnyi, I. Venevtsev, E. Gorokhova, S. Eron'ko, A. Chizhov, F. Muktepavela, Ultrafast luminescence of Ga- and In-doped ZnO ceramics, *Optical Materials: X* 12 (2021) 100106.
[DOI: 10.1016/j.omx.2021.100106](https://doi.org/10.1016/j.omx.2021.100106)
- [16] A. Bundulis, V. Kim, J. Grube, R. Ganeev, Nonlinear refraction and absorption of spectrally tuneable picosecond pulses in carbon disulfide, *Optical Materials* 122 (2021) 111778.
[DOI: 10.1016/j.optmat.2021.111778](https://doi.org/10.1016/j.optmat.2021.111778)
- [17] A. Lushchik, V. Kuzovkov, E. Kotomin, G. Prieditis, V. Seeman, E. Shablonin, E. Vasil'chenko, A. Popov, Evidence for the formation of two types of oxygen interstitials in neutron-irradiated α -Al₂O₃ single crystals, *Scientific Reports* 11 (2021) 20909.
[DOI: 10.1038/s41598-021-00336-0](https://doi.org/10.1038/s41598-021-00336-0)
- [18] M. Vanags, L. Mežule, A. Spule, J. Kostjukovs, K. Šmits, A. Tamm, T. Juhna, S. Vihodceva, T. Käämbre, L. Baumane, D. Začs, G. Vasiliev, M. Turks, I. Mierina, P. Sherrell, A. Šutka, Rapid catalytic water disinfection from earth abundant Ca₂Fe₂O₅ brownmillerite, *Advanced Sustainable Systems* 5 (2021) 2100130.
[DOI: 10.1002/adsu.202100130](https://doi.org/10.1002/adsu.202100130)
- [19] M. Gužauskas, E. Narbutaitis, D. Volyniuk, G. Baryshnikov, B. Minaev, H. Ågren, Y.-C. Chao, C.-C. Chang, M. Rutkis, J. Grazulevicius, Polymorph acceptor-based triads with photoinduced TADF for UV sensing, *Chemical Engineering Journal* 425 (2021) 131549.
[DOI: 10.1016/j.cej.2021.131549](https://doi.org/10.1016/j.cej.2021.131549)
- [20] J. Purans, A. Menushenkov, S. Besedin, A. Ivanov, V. Minkov, I. Pudza, A. Kuzmin, K. Klementiev, S. Pascarelli, O. Mathon, A. Rosa, T. Irifune, M. Eremets, Local electronic structure rearrangements and strong anharmonicity in YH₃ under pressures up to 180 GPa, *Nature Communications* 12 (2021) 1765.
[DOI: 10.1038/s41467-021-21991-x](https://doi.org/10.1038/s41467-021-21991-x)
- [21] P. Ščajev, R. Durena, P. Onufrijevs, S. Miasojedovas, T. Malinauskas, S. Stanionyte, A. Zarkov, A. Zukuls, I. Bite, K. Smits, Morphological and optical property study of Li doped ZnO produced by microwave-assisted solvothermal synthesis, *Materials Science in Semiconductor Processing* 135 (2021) 106069.

- [DOI: 10.1016/j.mssp.2021.106069](https://doi.org/10.1016/j.mssp.2021.106069)
- [22] G. Snarskis, J. Pilipavičius, D. Gryaznov, L. Mikoliū Naitė, L. Vilčiauskas, Peculiarities of phase formation in mn-based na superionic conductor (nasicon) systems: The case of $\text{Na}_{1+2x}\text{Mn}_x\text{Ti}_{2-x}(\text{PO}_4)_3$ ($0.0 \leq x \leq 1.5$), *Chemistry of Materials* 33 (2021) 8394–8403.
- [DOI: 10.1021/acs.chemmater.1c02775](https://doi.org/10.1021/acs.chemmater.1c02775)
- [23] B. Straumal, A. Korneva, A. Kuzmin, G. Lopez, E. Rabkin, A. Straumal, G. Gerstein, A. Gornakova, The grain boundary wetting phenomena in the Ti-containing high-entropy alloys: A review, *Metals* 11 (2021) 1881.
- [DOI: 10.3390/met11111881](https://doi.org/10.3390/met11111881)
- [24] M. Sokolov, Y. Mastrikov, G. Zvejnieks, D. Bocharov, E. Kotomin, V. Krasnenko, Water splitting on multifaceted SrTiO_3 nanocrystals: Computational study, *Catalysts* 11 (2021) 1326.
- [DOI: 10.3390/catal11111326](https://doi.org/10.3390/catal11111326)
- [25] Y.-P. Lin, I. Isakoviča, A. Gopejenko, A. Ivanova, A. Začinskis, R. Eglitis, P. D'yachkov, S. Piskunov, Time-dependent density functional theory calculations of n- and s-doped TiO_2 nanotube for water-splitting applications, *Nanomaterials* 11 (2021) 2900.
- [DOI: 10.3390/nano11112900](https://doi.org/10.3390/nano11112900)
- [26] L. Trinkler, A. Trukhin, J. Cipa, B. Berzina, UV light induced processes in pure and doped AlN ceramics, *Optical Materials* 121 (2021) 111550.
- [DOI: 10.1016/j.optmat.2021.111550](https://doi.org/10.1016/j.optmat.2021.111550)
- [27] N. Mironova-Ulmane, M. Brik, J. Grube, G. Krieke, A. Antuzevics, V. Skvortsova, M. Kemere, E. Elsts, A. Sarakovskis, M. Piasecki, A. Popov, Spectroscopic studies of Cr^{3+} ions in natural single crystal of magnesium aluminate spinel MgAl_2O_4 , *Optical Materials* 121 (2021) 111496.
- [DOI: 10.1016/j.optmat.2021.111496](https://doi.org/10.1016/j.optmat.2021.111496)
- [28] E. Butanovs, A. Zolotarjovs, A. Kuzmin, B. Polyakov, Nanoscale X-ray detectors based on individual CdS, SnO_2 and ZnO nanowires, *Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 1014 (2021) 165736.
- [DOI: 10.1016/j.nima.2021.165736](https://doi.org/10.1016/j.nima.2021.165736)
- [29] T. Akopdzhanyan, A. Kondakov, S. Rupasov, A. Kozlova, V. Pankratov, Optical properties of powder and ceramics of aluminium oxynitride obtained by self-propagating high-temperature synthesis, *Lithuanian Journal of Physics* 61 (2021) 169–176.
- [DOI: 10.3952/physics.v61i3.4516](https://doi.org/10.3952/physics.v61i3.4516)
- [30] V. Utochnikova, A. Aslandukov, A. Vashchenko, A. Goloveshkin, A. Alexandrov, R. Grzibovskis, J.-C. Bünzli, Identifying lifetime as one of the key parameters responsible for the low brightness of lanthanide-based OLEDs, *Dalton Transactions* 50 (2021) 12806–12813.
- [DOI: 10.1039/d1dt02269e](https://doi.org/10.1039/d1dt02269e)
- [31] L. Bikse, M. Dunce, E. Birks, K. Kundzins, O. Freimanis, M. Livins, J. Gabrusenoks, A. Sternberg, Impact of thermal treatment on the surface of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ -based ceramics, *Crystals* 11 (2021) 1266.
- [DOI: 10.3390/cryst11101266](https://doi.org/10.3390/cryst11101266)
- [32] R. Eglitis, J. Purans, A. Popov, R. Jia, Tendencies in ABO_3 perovskite and SrF_2 , BaF_2 and CaF_2 bulk and surface f-center ab initio computations at high symmetry cubic structure, *Symmetry* 13 (2021) 1920.
- [DOI: 10.3390/sym13101920](https://doi.org/10.3390/sym13101920)

- [33] S. Piskunov, A. Gopejenko, V. Pankratov, I. Isakoviča, C.-G. Ma, M. Brik, M. Piasecki, A. Popov, First principles calculations of atomic and electronic structure of Ti^{3+} - and Ti^{2+} -doped $YAlO_3$, *Materials* 14 (2021) 5589.
[DOI: 10.3390/ma14195589](https://doi.org/10.3390/ma14195589)
- [34] M. Norkus, M. Skruodienė, G. Niaura, A. Šarakovskis, R. Skaudžius, New low-temperature phosphate glasses as a host for europium ions, *Journal of Non-Crystalline Solids* 569 (2021) 120966.
[DOI: 10.1016/j.jnoncrysol.2021.120966](https://doi.org/10.1016/j.jnoncrysol.2021.120966)
- [35] G. Bakradze, A. Kalinko, A. Kuzmin, Evidence of nickel ions dimerization in $NiWO_4$ and $NiWO_4$ - $ZnWO_4$ solid solutions probed by EXAFS spectroscopy and reverse Monte Carlo simulations, *Acta Materialia* 217 (2021) 117171.
[DOI: 10.1016/j.actamat.2021.117171](https://doi.org/10.1016/j.actamat.2021.117171)
- [36] G. Inkrataite, M. Kemere, A. Sarakovskis, R. Skaudžius, Influence of boron on the essential properties for new generation scintillators, *Journal of Alloys and Compounds* 875 (2021) 160002.
[DOI: 10.1016/j.jallcom.2021.160002](https://doi.org/10.1016/j.jallcom.2021.160002)
- [37] D. Bocharov, I. Pudza, K. Klementiev, M. Krack, A. Kuzmin, Study of high-temperature behaviour of zno by ab initio molecular dynamics simulations and x-ray absorption spectroscopy, *Materials* 14 (2021) 5206.
[DOI: 10.3390/ma14185206](https://doi.org/10.3390/ma14185206)
- [38] F. Gentile, R. Diana, B. Panunzi, U. Caruso, A. Platonenko, F. Pascale, R. Dovesi, Vibrational analysis of paraelectric–ferroelectric transition of $LiNbO_3$: An ab-initio quantum mechanical treatment, *Symmetry* 13 (2021) 1650.
[DOI: 10.3390/sym13091650](https://doi.org/10.3390/sym13091650)
- [39] K. Chernenko, A. Kivimäki, R. Pärna, W. Wang, R. Sankari, M. Leandersson, H. Tarawneh, V. Pankratov, M. Kook, E. Kukk, Reisberg, S. Urpelainen, T. Käämbre, F. Siewert, G. Gwalt, A. Sokolov, S. Lemke, S. Alimov, J. Knedel, O. Kutz, T. Seliger, M. Valden, Hirsimäki, M. Kirm, M. Huttula, Performance and characterization of the FinEstBeAMS beamline at the MAX IV Laboratory, *Journal of Synchrotron Radiation* 28 (2021) 1620–1630.
[DOI: 10.1107/S1600577521006032](https://doi.org/10.1107/S1600577521006032)
- [40] S. Samanta, A. Nissimagoudar, R. Basori, A. Kuzmin, M. Li, J. Zhang, L. Wang, Y. Tian, H.-K. Mao, Unprecedented pressure-driven metallization and topological charge transport in an anion radical salt, *Materials Today Physics* 20 (2021) 100467.
[DOI: 10.1016/j.mtphys.2021.100467](https://doi.org/10.1016/j.mtphys.2021.100467)
- [41] I. Pudza, A. Anspoks, A. Cintins, A. Kalinko, E. Welter, A. Kuzmin, The influence of Zn^{2+} ions on the local structure and thermochromic properties of $Cu_{1-x}Zn_xMoO_4$ solid solutions, *Materials Today Communications* 28 (2021) 102607.
[DOI: 10.1016/j.mtcomm.2021.102607](https://doi.org/10.1016/j.mtcomm.2021.102607)
- [42] G. Krieke, A. Antuzevics, B. Berzina, Defect formation in photochromic $Ca_2SnO_4:Al^{3+}$, *Materials Today Communications* 28 (2021) 102592.
[DOI: 10.1016/j.mtcomm.2021.102592](https://doi.org/10.1016/j.mtcomm.2021.102592)
- [43] V. Khanin, I. Venevtsev, K. Chernenko, V. Pankratov, K. Klementiev, T. van Swieten, A. van Bunningen, I. Vrabel, R. Shendrik, C. Ronda, P. Rodnyi, A. Meijerink, Exciton interaction with Ce^{3+}

and Ce⁴⁺ ions in (LuGd)₃(Ga,Al)₅O₁₂ ceramics, Journal of Luminescence 237 (2021) 118150.

[DOI: 10.1016/j.jlumin.2021.118150](https://doi.org/10.1016/j.jlumin.2021.118150)

- [44] E. Feldbach, L. Museur, V. Krasnenko, A. Zerr, M. Kitaura, A. Kanaev, Defects induced by He+ irradiation in γ -Si₃N₄, Journal of Luminescence 237 (2021) 118132.
[DOI: 10.1016/j.jlumin.2021.118132](https://doi.org/10.1016/j.jlumin.2021.118132)
- [45] B. Garbarz-Glos, W. Bak, M. Antonova, A. Kalvane, C. Kajtoch, P. Dulian, Influence of cation order on the dielectric properties of (1-x)Pb(Sc_{0.5}Nb_{0.5})O₃-xPb(Yb_{0.5}Nb_{0.5})O₃ ceramics, Materials Science - Poland 38 (2021) 402–406.
[DOI: 10.2478/msp-2020-0058](https://doi.org/10.2478/msp-2020-0058)
- [46] G. Zvejnieks, D. Zavickis, E. Kotomin, D. Gryaznov, BaCoO₃ monoclinic structure and chemical bonding analysis: Hybrid DFT calculations, Physical Chemistry Chemical Physics 23 (2021) 17493–17501.
[DOI: 10.1039/d1cp01900g](https://doi.org/10.1039/d1cp01900g)
- [47] F. Murzakhanov, P. Grishin, M. Goldberg, B. Yavkin, G. Mamin, S. Orlinskii, A. Fedotov, N. Petrakova, A. Antuzevics, M. Gafurov, V. Komlev, Radiation-induced stable radicals in calcium phosphates: Results of multifrequency EPR, EDNMR, ESEEM, and ENDOR studies, Applied Sciences (Switzerland) 11 (2021) 7727.
[DOI: 10.3390/app11167727](https://doi.org/10.3390/app11167727)
- [48] A. Plavniece, A. Volperts, G. Dobeles, A. Zhurinsh, K. Kaare, Kruusenbergs, K. Kaprans, A. Knoks, J. Kleperis, Wood and black liquor-based n-doped activated carbon for energy application, Sustainability (Switzerland) 13 (2021) 9237.
[DOI: 10.3390/su13169237](https://doi.org/10.3390/su13169237)
- [49] Y. Fu, T. Yager, G. Chikvaidze, S. Iyer, Q. Wang, Time-resolved FDTD and experimental FTIR study of gold micropatch arrays for wavelength-selective mid-infrared optical coupling, Sensors 21 (2021) 5203.
[DOI: 10.3390/s21155203](https://doi.org/10.3390/s21155203)
- [50] O. Lisovski, S. Piskunov, D. Bocharov, S. Kenmoe, 2d slab models of nanotubes based on tetragonal TiO₂ structures: Validation over a diameter range, Nanomaterials 11 (2021) 1925.
[DOI: 10.3390/nano11081925](https://doi.org/10.3390/nano11081925)
- [51] M. Rudysh, P. Shchepanskyi, A. Fedorchuk, M. Brik, V. Stadnyk, G. Myronchuk, E. Kotomin, M. Piasecki, Impact of anionic system modification on the desired properties for CuGa(S_{1-x}Se_x)₂ solid solutions, Computational Materials Science 196 (2021) 110553.
[DOI: 10.1016/j.commatsci.2021.110553](https://doi.org/10.1016/j.commatsci.2021.110553)
- [52] L. Skuja, N. Ollier, K. Kajihara, I. Bite, M. Leimane, K. Smits, A. Silins, Optical absorption of excimer laser-induced dichlorine monoxide in silica glass and excitation of singlet oxygen luminescence by energy transfer from chlorine molecules, Physica Status Solidi (A) Applications and Materials Science 218 (2021) 2100009.
[DOI: 10.1002/pssa.202100009](https://doi.org/10.1002/pssa.202100009)
- [53] F. Correia, J. Ribeiro, A. Kuzmin, I. Pudza, A. Kalinko, E. Welter, A. Mendes, J. Rodrigues, N. Sedrine, T. Monteiro, M. Correia, C. Tavares, The role of Ga and Bi doping on the local structure of transparent zinc oxide thin films, Journal of Alloys and Compounds 870 (2021) 159489.

[DOI: 10.1016/j.jallcom.2021.159489](https://doi.org/10.1016/j.jallcom.2021.159489)

- [54] D. Griesiute, L. Sinusaite, A. Kizalaite, A. Antuzevics, K. Mazeika, D. Baltrunas, T. Goto, T. Sekino, A. Kareiva, A. Zarkov, The influence of Fe³⁺ doping on thermally induced crystallization and phase evolution of amorphous calcium phosphate, *CrystEngComm* 23 (2021) 4627–4637.
[DOI: 10.1039/d1ce00371b](https://doi.org/10.1039/d1ce00371b)
- [55] A. Šutka, M. Zubkins, A. Linarts, L. Lapčinskis, K. Malnieks, O. Verners, A. Sarakovskis, R. Grzibovskis, J. Gabrusenoks, E. Strods, K. Smits, V. Vibornijs, L. Bikse, J. Purans, Tribovoltaic device based on the W/WO₃ schottky junction operating through hot carrier extraction, *Journal of Physical Chemistry C* 125 (2021) 14212–14220.
[DOI: 10.1021/acs.jpcc.1c04312](https://doi.org/10.1021/acs.jpcc.1c04312)
- [56] T. Tsebriienko, A. Popov, Effect of poly (Titanium oxide) on the viscoelastic and thermophysical properties of interpenetrating polymer networks, *Crystals* 11 (2021) 794.
[DOI: 10.3390/cryst11070794](https://doi.org/10.3390/cryst11070794)
- [57] A. Antuzevics, G. Kriekē, H. Ozols, A. Fedotovs, A. Sarakovskis, A. Kuzmin, Oxidation state and local structure of chromium ions in LaOCl, *Materials* 14 (2021) 3539.
[DOI: 10.3390/ma14133539](https://doi.org/10.3390/ma14133539)
- [58] V. Serga, R. Burve, A. Krumina, V. Pankratova, A. Popov, V. Pankratov, Study of phase composition, photocatalytic activity, and photoluminescence of TiO₂ with Eu additive produced by the extraction-pyrolytic method, *Journal of Materials Research and Technology* 13 (2021) 2350–2360.
[DOI: 10.1016/j.jmrt.2021.06.029](https://doi.org/10.1016/j.jmrt.2021.06.029)
- [59] E. Feldbach, A. Zerr, L. Museur, M. Kitaura, G. Manthilake, F. Tessier, Krasnenko, A. Kanaev, Electronic band transitions in γ-Ge₃N₄, *Electronic Materials Letters* 17 (2021) 315–323.
[DOI: 10.1007/s13391-021-00291-y](https://doi.org/10.1007/s13391-021-00291-y)
- [60] S. Ratso, P. Walke, V. Mikli, J. Ločs, K. Šmits, V. Vītola, A. Šutka, Kruusenbergs, CO₂ turned into a nitrogen doped carbon catalyst for fuel cells and metal-air battery applications, *Green Chemistry* 23 (2021) 4435–4445.
[DOI: 10.1039/d1gc00659b](https://doi.org/10.1039/d1gc00659b)
- [61] I. Kužniarska-Biernacka, B. Garbarz-Glos, E. Skiba, W. Maniukiewicz, Bak, M. Antonova, S. Rebelo, C. Freire, Evaluation of rhodamine b photocatalytic degradation over BaTiO₃-MnO₂ ceramic materials, *Materials* 14 (2021) 3152.
[DOI: 10.3390/ma14123152](https://doi.org/10.3390/ma14123152)
- [62] M. Bisztyga-Szklarz, K. Mech, M. Marzec, R. Kalendarev, K. Szacilowski, In situ regeneration of copper-coated gas diffusion electrodes for electroreduction of CO₂ to ethylene, *Materials* 14 (2021) 3171.
[DOI: 10.3390/ma14123171](https://doi.org/10.3390/ma14123171)
- [63] J. Kleperis, D. Boss, A. Mezulis, L. Zemite, P. Lesnicenoks, A. Knoks, L. Dimanta, Analysis of the Role of the Latvian Natural Gas Network for the use of Future Energy Systems: Hydrogen from Res, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 214–226.
[DOI: 10.2478/lpts-2021-0027](https://doi.org/10.2478/lpts-2021-0027)
- [64] G. Doke, A. Antuzevics, G. Kriekē, A. Kalnina, M. Springis, A. Sarakovskis, UV and X-ray excited red persistent luminescence in Mn²⁺ doped MgGeO₃ material synthesized in air and reducing

atmosphere, *Journal of Luminescence* 234 (2021) 117995.

[DOI: 10.1016/j.jlumin.2021.117995](https://doi.org/10.1016/j.jlumin.2021.117995)

- [65] B. Zhang, M. Clausi, B. Heck, S. Laurenzi, M. Santonicola, J. Kleperis, A. Antuzevičs, G. Reiter, A. Aleshin, A. Lobach, Changes in surface free energy and surface conductivity of carbon nanotube/polyimide nanocomposite films induced by uv irradiation, *ACS Applied Materials and Interfaces* 13 (2021) 24218–24227.

[DOI: 10.1021/acsami.1c02654](https://doi.org/10.1021/acsami.1c02654)

- [66] A. Ivanova, A. Chesnokov, D. Bocharov, K. Exner, A universal approach to quantify overpotential-dependent selectivity trends for the competing oxygen evolution and peroxide formation reactions: a case study on graphene model electrodes, *Journal of Physical Chemistry C* 125 (2021) 10413–10421.

[DOI: 10.1021/acs.jpcc.1c03323](https://doi.org/10.1021/acs.jpcc.1c03323)

- [67] A. Platonenko, F. Colasuonno, F. Gentile, F. Pascale, R. Dovesi, Oxygen and vacancy defects in silicon. A quantum mechanical characterization through the IR and Raman spectra, *Journal of Chemical Physics* 154 (2021) 174707.

[DOI: 10.1063/5.0044106](https://doi.org/10.1063/5.0044106)

- [68] A. Platonenko, F. Gentile, F. Pascale, P. D'Arco, R. Dovesi, Interstitial carbon defects in silicon. A quantum mechanical characterization through the infrared and Raman spectra, *Journal of Computational Chemistry* 42 (2021) 806–817.

[DOI: 10.1002/jcc.26500](https://doi.org/10.1002/jcc.26500)

- [69] I. Ristić, A. Miletić, N. Vukić, M. Marinović-Cincović, K. Smits, S. Cakić, B. Pilić, Characterization of electrospun poly(lactide) composites containing multiwalled carbon nanotubes, *Journal of Thermoplastic Composite Materials* 34 (2021) 695–706.

[DOI: 10.1177/0892705719857780](https://doi.org/10.1177/0892705719857780)

- [70] D.-C. Yang, Y.-B. Tan, R. Eglitis, S. Bibi, R. Jia, H.-X. Zhang, Dipoles in 4,12,4-graphyne, *Applied Surface Science* 545 (2021) 148991.

[DOI: 10.1016/j.apsusc.2021.148991](https://doi.org/10.1016/j.apsusc.2021.148991)

- [71] A. Chesnokov, D. Gryaznov, N. Skorodumova, E. Kotomin, A. Zitolo, M. Zubkins, A. Kuzmin, A. Anspoks, J. Purans, The local atomic structure and thermoelectric properties of Ir-doped ZnO: hybrid DFT calculations and XAS experiments, *Journal of Materials Chemistry C* 9 (2021) 4948–4960.

[DOI: 10.1039/d1tc00223f](https://doi.org/10.1039/d1tc00223f)

- [72] L. Lapčinskis, A. Linarts, K. Malnieks, H. Kim, K. Rubenis, K. Pudzs, K. Smits, A. Kovalovs, K. Kalniņš, A. Tamm, C. Jeong, A. Šutka, Triboelectrification of nanocomposites using identical polymer matrixes with different concentrations of nanoparticle fillers, *Journal of Materials Chemistry A* 9 (2021) 8984–8990.

[DOI: 10.1039/d0ta12441a](https://doi.org/10.1039/d0ta12441a)

- [73] K. Traskovskis, A. Sebris, I. Novosjolova, M. Turks, M. Guzauskas, D. Volyniuk, O. Bezvikonnyi, J. Grazulevicius, A. Mishnev, R. Grzibovskis, A. Vembris, All-organic fast intersystem crossing assisted exciplexes exhibiting sub-microsecond thermally activated delayed fluorescence, *Journal of Materials Chemistry C* 9 (2021) 4532–4543.

[DOI: 10.1039/d0tc05099g](https://doi.org/10.1039/d0tc05099g)

- [74] R. Eglitis, J. Purans, R. Jia, Comparative hybrid Hartree-Fock-DFT calculations of WO₂-terminated cubic WO₃ as well as SrTiO₃, BaTiO₃, PbTiO₃ and CaTiO₃ (001) surfaces, *Crystals* 11 (2021) 455.
[DOI: 10.3390/cryst11040455](https://doi.org/10.3390/cryst11040455)
- [75] A. Usseinov, Z. Koishybayeva, A. Platonenko, A. Akilbekov, J. Purans, V. Pankratov, Y. Suchikova, A. Popov, Ab-Initio calculations of oxygen vacancy in Ga₂O₃ crystals, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 3–10.
[DOI: 10.2478/lpts-2021-0007](https://doi.org/10.2478/lpts-2021-0007)
- [76] S. Kato, N. Nakajima, S. Yasui, S. Yasuhara, D. Fu, J. Adachi, H. Nitani, Y. Takeichi, A. Anspoks, Dielectric response of BaTiO₃ electronic states under AC fields via microsecond time-resolved X-ray absorption spectroscopy, *Acta Materialia* 207 (2021) 116681.
[DOI: 10.1016/j.actamat.2021.116681](https://doi.org/10.1016/j.actamat.2021.116681)
- [77] G. Krucaite, D. Tavgeniene, D. Blazevicius, B. Zhang, A. Vembris, S. Grigalevicius, New electroactive polymers with electronically isolated 4,7-diarylfuorene chromophores as positive charge transporting layer materials for OLEDs, *Molecules* 26 (2021) 1936.
[DOI: 10.3390/molecules26071936](https://doi.org/10.3390/molecules26071936)
- [78] A. Šutka, R. Eglitis, A. Kuzma, K. Smits, A. Zukuls, J. Prades, C. Fàbrega, Photodoping-inspired room-temperature gas sensing by anatase TiO₂ quantum dots, *ACS Applied Nano Materials* 4 (2021) 2522–2527.
[DOI: 10.1021/acsnm.0c03089](https://doi.org/10.1021/acsnm.0c03089)
- [79] S. Vihodceva, A. Šutka, M. Sihtmäe, M. Rosenberg, M. Otsus, I. Kurvet, K. Smits, L. Bikse, A. Kahru, K. Kasemets, Antibacterial activity of positively and negatively charged hematite (α-Fe₂O₃) nanoparticles to escherichia coli, staphylococcus aureus and vibrio fischeri, *Nanomaterials* 11 (2021) 652.
[DOI: 10.3390/nano11030652](https://doi.org/10.3390/nano11030652)
- [80] O. Petrichenko, A. Plotniece, K. Pajuste, M. Rucins, P. Dimitrijevs, A. Sobolev, E. Sprugis, A. Cēbers, Evaluation of physicochemical properties of amphiphilic 1,4-dihydropyridines and preparation of magnetoliposomes, *Nanomaterials* 11 (2021) 593.
[DOI: 10.3390/nano11030593](https://doi.org/10.3390/nano11030593)
- [81] G. Kriekē, A. Antuzevics, K. Smits, D. Millers, Enhancement of persistent luminescence in Ca₂SnO₄:Sm³⁺, *Optical Materials* 113 (2021) 110842.
[DOI: 10.1016/j.optmat.2021.110842](https://doi.org/10.1016/j.optmat.2021.110842)
- [82] J. Andzane, A. Felsharuk, A. Sarakovskis, U. Malinovskis, E. Kauranens, M. Bechelany, K. Niherysh, I. Komissarov, D. Erts, Thickness-dependent properties of ultrathin bismuth and antimony chalcogenide films formed by physical vapor deposition and their application in thermoelectric generators, *Materials Today Energy* 19 (2021) 100587.
[DOI: 10.1016/j.mtener.2020.100587](https://doi.org/10.1016/j.mtener.2020.100587)
- [83] R. Olins, P. Lesnicenoks, J. Kleperis, A. Knoks, I. Lukosevics, Electrochemical exfoliation-streamline method for synthesis of nitrogen doped graphene, *Chemija* 32 (2021) 9–16.
[DOI: 10.6001/CHEMIJA.V32I1.4396](https://doi.org/10.6001/CHEMIJA.V32I1.4396)
- [84] E. Zarins, J. Pervenecka, E. Misina, O. Bezvikonnyi, A. Vembris, K. Balodis, D. Volyniuk, J. Grazulevicius, V. Kokars, HAPPY dyes as light amplification media in thin films, *Journal of Organic*

Chemistry 86 (2021) 3213–3222.

[DOI: 10.1021/acs.joc.0c02574](https://doi.org/10.1021/acs.joc.0c02574)

- [85] I. Pudza, A. Kalinko, A. Cintins, A. Kuzmin, Study of the thermochromic phase transition in $\text{CuMo}_{1-x}\text{W}_x\text{O}_4$ solid solutions at the W L_3 -edge by resonant X-ray emission spectroscopy, *Acta Materialia* 205 (2021) 116581.
[DOI: 10.1016/j.actamat.2020.116581](https://doi.org/10.1016/j.actamat.2020.116581)
- [86] L. Sinusaite, A. Antuzevics, A. Popov, U. Rogulis, M. Misevicius, A. Katelnikovas, A. Kareiva, A. Zarkov, Synthesis and luminescent properties of Mn-doped alpha-tricalcium phosphate, *Ceramics International* 47 (2021) 5335–5340.
[DOI: 10.1016/j.ceramint.2020.10.114](https://doi.org/10.1016/j.ceramint.2020.10.114)
- [87] M. Tyunina, L. Rusevich, E. Kotomin, O. Pacherova, T. Kocourek, A. Dejneka, Epitaxial growth of perovskite oxide films facilitated by oxygen vacancies, *Journal of Materials Chemistry C* 9 (2021) 1693–1700.
[DOI: 10.1039/d0tc05750a](https://doi.org/10.1039/d0tc05750a)
- [88] A. Supe, S. Olonkins, A. Udalcovs, U. Senkans, R. Murnieks, L. Gegere, D. Prigunovs, J. Grube, E. Elsts, S. Spolitis, O. Ozolins, V. Bobrovs, Cladding-pumped erbium/ytterbium co-doped fiber amplifier for c- band operation in optical networks, *Applied Sciences (Switzerland)* 11 (2021) 1702.
[DOI: 10.3390/app11041702](https://doi.org/10.3390/app11041702)
- [89] V. Malgin, O. Yakovlev, L. Skuja, Improvement of vacuum characteristics of cryostats for HPGe gamma-radiation detectors, *Journal of Instrumentation* 16 (2021) P02012.
[DOI: 10.1088/1748-0221/16/02/P02012](https://doi.org/10.1088/1748-0221/16/02/P02012)
- [90] J. Cipa, L. Trinkler, B. Berzina, Thermoluminescence response of $\text{AlN}+\text{Y}_2\text{O}_3$ ceramics to sunlight and X-ray irradiation, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 3–14.
[DOI: 10.2478/lpts-2021-0001](https://doi.org/10.2478/lpts-2021-0001)
- [91] E. Einbergs, A. Zolotarjovs, I. Bite, J. Cipa, V. Vitola, K. Laganovska, L. Trinkler, Re-evaluation of chromium doped alumina for dosimetric applications, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 15–22.
[DOI: 10.2478/lpts-2021-0002](https://doi.org/10.2478/lpts-2021-0002)
- [92] I. Kaulachs, A. Ivanova, A. Holsts, M. Roze, A. Flerov, A. Tokmakov, Mihailovs, M. Rutkis, Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$ solar cells. Experimental study of initial degradation kinetics and fill factor spectral dependence, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 53–69.
[DOI: 10.2478/lpts-2021-0006](https://doi.org/10.2478/lpts-2021-0006)
- [93] A. Spustaka, M. Senko, D. Millers, I. Bite, K. Smits, V. Vitola, Gallium Concentration Optimisation of Gallium Doped Zinc Oxide for Improvement of Optical Properties, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 33–43.
[DOI: 10.2478/lpts-2021-0004](https://doi.org/10.2478/lpts-2021-0004)
- [94] I. Kaulachs, A. Ivanova, A. Tokmakov, M. Roze, I. Mihailovs, M. Rutkis, Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$ solar cells and their degradation (Part 1: A Short Review), *Latvian Journal of Physics and Technical Sciences* 58 (2021) 44–52.
[DOI: 10.2478/lpts-2021-0005](https://doi.org/10.2478/lpts-2021-0005)

- [95] F. Muktepavela, A. Zolotarjovs, R. Zabels, K. Kundzins, E. Gorokhova, E. Tamanis, Comparative study on micromechanical properties of ZnO:Ga and ZnO:In luminescent Ceramics, *Latvian Journal of Physics and Technical Sciences* 58 (2021) 23–32.
DOI: [10.2478/lpts-2021-0003](https://doi.org/10.2478/lpts-2021-0003)
- [96] D. Shurtakova, B. Yavkin, G. Mamin, S. Orlinskii, V. Sirotinkin, A. Fedotov, A. Shinkarev, A. Antuzevics, I. Smirnov, V. Tovtin, E. Starostin, Gafurov, V. Komlev, X-ray diffraction and multifrequency epr study of radiation-induced room temperature stable radicals in octacalcium phosphate, *Radiation Research* 195 (2021) 200–210.
DOI: [10.1667/RADE-20-00194.1](https://doi.org/10.1667/RADE-20-00194.1)
- [97] A. Laurikenas, D. Sakalauskas, A. Marsalka, R. Raudonis, A. Antuzevics, V. Balevicius, A. Zarkov, A. Kareiva, Investigation of lanthanum substitution effects in yttrium aluminium garnet: importance of solid state NMR and EPR methods, *Journal of Sol-Gel Science and Technology* 97 (2021) 479–487.
DOI: [10.1007/s10971-020-05445-2](https://doi.org/10.1007/s10971-020-05445-2)
- [98] S. Khartsev, N. Nordell, M. Hammar, J. Purans, A. Hallen, High-quality Si-Doped β -Ga₂O₃ films on sapphire fabricated by pulsed laser deposition, *Physica Status Solidi (B) Basic Research* 258 (2021) 2000362.
DOI: [10.1002/pssb.202000362](https://doi.org/10.1002/pssb.202000362)
- [99] P. Fu, D.-C. Yang, R. Jia, Z.-J. Yi, Z.-F. Liu, X. Li, R. Eglitis, Z.-M. Su, Metallic subnanometer porous silicon: A theoretical prediction, *Physical Review B* 103 (2021) 014117.
DOI: [10.1103/PhysRevB.103.014117](https://doi.org/10.1103/PhysRevB.103.014117)
- [100] A. Dauletbekova, V. Skuratov, E. Kotomin, A. Popov, Preface, *Nuclear Instruments and Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms* 487 (2021) 96.
DOI: [10.1016/j.nimb.2020.11.003](https://doi.org/10.1016/j.nimb.2020.11.003)
- [101] E. Butanovs, A. Kuzmin, S. Piskunov, K. Smits, A. Kalinko, B. Polyakov, Synthesis and characterization of GaN/ReS₂, ZnS/ReS₂ and ZnO/ReS₂ core/shell nanowire heterostructures, *Applied Surface Science* 536 (2021) 147841.
DOI: [10.1016/j.apsusc.2020.147841](https://doi.org/10.1016/j.apsusc.2020.147841)
- [102] E. Zarins, D. Alksnis, P. Paulsone, K. Balodis, A. Vembris, V. Kokars, Synthesis and spectroscopic characteristics of ligands based on quinolin-8-ol as useful precursors for alq3 type complexes, *Key Engineering Materials* 903 KEM (2021) 168–173.
DOI: [10.4028/www.scientific.net/KEM.903.168](https://doi.org/10.4028/www.scientific.net/KEM.903.168)
- [103] R. Eglitis, J. Purans, R. Jia, Comparative hybrid hartree-fock-dft calculations of ReO₃, SrTiO₃, BaTiO₃, PbTiO₃ and CaTiO₃ (001) surfaces, *Integrated Ferroelectrics* 220 (2021) 9–17.
DOI: [10.1080/10584587.2021.1921530](https://doi.org/10.1080/10584587.2021.1921530)
- [104] A. Bundulis, M. Rutkis, Z-scan extensions for inclusive study of nonlinear refractive index, *Optics InfoBase Conference Papers* (2021) NTh3A.21.
DOI: [10.1364/NLO.2021.NTh3A.21](https://doi.org/10.1364/NLO.2021.NTh3A.21)
- [105] A. Ozols, G. Mozolevskis, E. Letko, M. Rutkis, R. Zabels, E. Linina, Osmanis, Sputtered sioxny thin films – improving optical efficiency of liquid crystal diffuser elements in multi-focal near-to-eye display architecture, *Proc. SPIE* 11872 (2021) 118720I.
DOI: [10.1117/12.2596885](https://doi.org/10.1117/12.2596885)

- [106] A. Rucins, E. Straumite, D. Viesturs, A. Kristins, Studies of the possibilities to use ozone for the grain storage, *Vide. Tehnologija. Resursi-Environment, Technology, Resources* 3 (2021) 304–309.
[DOI: 10.17770/etr2021vol3.6519](https://doi.org/10.17770/etr2021vol3.6519)
- [107] V. Karitans, A. Tokmakovs, A. Antonuka, The effect of noise, a constant background, and bit depth on the phase retrieval of pure phase objects, *Optica Applicata* 51 (2021) 257–269.
[DOI: 10.37190/oa210209](https://doi.org/10.37190/oa210209)
- [108] V. Karitans, S. Fomins, M. Ozolinsh, Phase retrieval for studying the structure of vitreous floaters simulated in a model eye, *Journal of Modern Optics* 68 (2021) 792–797.
[DOI: 10.1080/09500340.2021.1948624](https://doi.org/10.1080/09500340.2021.1948624)
- [109] A. Bundulis, M. Rutkis, Interferometric Z-scan method for thermo-optical effect studies, *Proc. SPIE* 11770 (2021) 117701X.
[DOI: 10.1117/12.2593244](https://doi.org/10.1117/12.2593244)
- [110] E. Straumite, A. Rucins, D. Viesturs, J. Kleperis, A. Kristins, Evaluation of ozone influence on wheat grain quality during active drying, *Agronomy Research* 19 (2021) 1308–1317.
[DOI: 10.15159/AR.21.053](https://doi.org/10.15159/AR.21.053)
- [111] R. Rimsa, A. Galvanovskis, J. Plume, F. Rumnieks, K. Grindulis, G. Paidere, S. Erentraute, G. Mozolevskis, A. Abols, Lung on a chip development from off-stoichiometry thiol-ene polymer, *Micromachines* 12 (2021) 546.
[DOI: 10.3390/mi12050546](https://doi.org/10.3390/mi12050546)
- [112] A. Burkhanov, R. Dikov, K. Bormanis, The effect of bias field on the dielectric response of $\text{Ba}_{0.95}\text{Pb}_{0.05}\text{TiO}_3+\text{Co}_2\text{O}_3$, *Ferroelectrics* 574 (2021) 72–77.
[DOI: 10.1080/00150193.2021.1888050](https://doi.org/10.1080/00150193.2021.1888050)
- [113] V. Serga, R. Burve, A. Krumina, M. Romanova, E. Kotomin, A. Popov, Extraction–pyrolytic method for TiO_2 polymorphs production, *Crystals* 11 (2021) 431.
[DOI: 10.3390/cryst11040431](https://doi.org/10.3390/cryst11040431)
- [114] K. Nowak, O. Dumbrajs, Optimization of gyrotron resonator’s dimensions, *Journal of Telecommunications and Information Technology* 2021 (2021) 71–76.
[DOI: 10.26636/JTIT.2021.147120](https://doi.org/10.26636/JTIT.2021.147120)
- [115] A. Krauklis, C. Karl, A. Gagani, J. Jørgensen, Composite material recycling technology—state-of-the-art and sustainable development for the 2020s, *Journal of Composites Science* 5 (2021) 28.
[DOI: 10.3390/jcs5010028](https://doi.org/10.3390/jcs5010028)
- [116] X. Chen, G. Nusinovich, O. Dumbrajs, H. Xiao, D. Xia, T. Ding, L. Liu, Han, T. Peng, Shadowing of the operating mode by sidebands in gyrotrons with diode-type electron guns, *Physics of Plasmas* 28 (2021) 013110.
[DOI: 10.1063/5.0036054](https://doi.org/10.1063/5.0036054)
- [117] V. Vitola, I. Bite, I. Apsite, A. Zolotarjovs, A. Biswas, CuS/polyurethane composite appropriate for 4D printing, *Journal of Polymer Research* 28 (2021) 13.
[DOI: 10.1007/s10965-020-02375-z](https://doi.org/10.1007/s10965-020-02375-z)
- [118] R. Balakhayeva, A. Akilbekov, Z. Baimukhanov, A. Usseinov, S. Giniyatova, M. Zdorovets, L.

Vlasukova, A. Popov, A. Dauletbekova, CdTe Nanocrystal Synthesis in SiO₂/Si Ion-Track Template: The Study of Electronic and Structural Properties, *Physica Status Solidi (A) Applications and Materials Science* 218 (2021) 2000231.

[DOI: 10.1002/pssa.202000231](https://doi.org/10.1002/pssa.202000231)

[119] M. Paiders, V. Nikolajeva, G. Makarenkova, L. Orola, I. Dimanta, J. Kleperis, Changes in freshwater sediment microbial populations during fermentation of crude glycerol, *Electronic Journal of Biotechnology* 49 (2021) 34–41.

[DOI: 10.1016/j.ejbt.2020.10.007](https://doi.org/10.1016/j.ejbt.2020.10.007)

[120] E. Shablonin, A. Popov, G. Prieditis, E. Vasil'chenko, A. Lushchik, Thermal annealing and transformation of dimer F centers in neutron-irradiated Al₂O₃ single crystals, *Journal of Nuclear Materials* 543 (2021) 152600.

[DOI: 10.1016/j.jnucmat.2020.152600](https://doi.org/10.1016/j.jnucmat.2020.152600)

[121] V. Vitola, V. Lahti, I. Bite, A. Spustaka, D. Millers, M. Lastusaari, L. Petit, K. Smits, Low temperature afterglow from SrAl₂O₄: Eu, Dy, B containing glass, *Scripta Materialia* 190 (2021) 86–90.

[DOI: 10.1016/j.scriptamat.2020.08.023](https://doi.org/10.1016/j.scriptamat.2020.08.023)

[122] I. Pudza, A. Kuzmin, Treatment of disorder effects in X-ray absorption spectra by reverse Monte Carlo simulations: CuMoO₄ case, *Acta Crystallographica A* 77 (2021) C602.

Theses

Doctor Theses

No.	Author	Title	Supervisor	Degree
1.	A. Zolotarjovs	Optical properties of plasma electrolytic oxidation coatings on aluminium alloy surface	Dr. phys. K. Smits	Ph.D.

M.Sc. Theses

No.	Author	Title	Supervisor	Study programme
1.	M. Leimane	Preparation of monolithic silica by the sol-gel method	Dr. habil. phys. L. Skuja	Chemistry
2.	E. Einbergs	Applicability of mechanoluminescent materials for the development of optoelectric sensors and development of a method for the study of their properties	Dr. Phys. V. Vītola	Physics
3.	M. Lielbārdis	Selection of dielectric material of organic field effect transistor and determination of parameters	Dr. phys. A. Vembris	Physics
4.	I. Lukoševičs	Raman spectroscopy of white phosphorus alpha and beta phases	Dr. phys. J. Gabrusenoks	Physics
5.	J. Cīrulis	The incorporation of gadolinium ions into calcium fluoride oxyfluoride glass-ceramics is temperature dependent	Dr. phys. A. Antuzevičs	Physics
6.	D. Ņilova	Modulation of luminescence intensity with electric field based on $\text{Na}_{3.5}\text{Bi}_{0.5}\text{TiO}_3$ activated compound with Er^{3+} and Yb^{3+}	Ph.D. G.Krieķe, Dr.phys. Ē. Birks	Physics
7.	J. Čīpa	Investigation of luminescence properties of alloyed AlN ceramics	Dr. phys. L. Trinklere	Physics
8.	M. K. Jurjāns	Investigation of electromechanical properties in ferroelectric compounds based on NBT	Dr. Phys. Ē. Birks	Physics

B.Sc. Theses

No.	Author	Title	Supervisor	Study programme
1.	J. Sušinska	Thermal annealing effect on the structure of LiF single crystals irradiated with swift ³⁶ S ions	Mg. phys. L. Bikše	Chemistry
2.	L. Dipāne	Cadmium sulfide nanowire surface passivation to reduce environmental degradation	Dr. phys. E. Butanovs	Chemistry
3.	S. Homiča	SPEEK composite membranes for sodium ion batteries	Dr.chem. G. Vaivars	Chemistry
4.	M. Dile	Synthesis of manganese-doped zinc sulfide nanomaterials	Mg. K. Laganovska	Chemistry
5.	V. Paramonova	Holographic recording azobenzene DO-3 and epoxide synthesis	Dr.phys. J. Teteris	Chemistry
6.	A. Spustaka	Luminescent properties of zinc oxide	Dr. phys. V. Vītola	Physics
7.	A. Bērziņa	Development of SU-8 waveguide optical gas sensor with optical lithography technique and characterization of its optical properties	Ph.D. A. Bundulis	Physics
8.	M.A. Zommere	Optical studies of difensulfones and benzophenone derivatives for 3rd generation organic light emitting diodes	Dr. phys. A. Vembris	Physics
9.	O.M. Eberliņš	Electrocaloric effect in ferroelectrics with perovskite structure at a large electric field	Dr. Phys. Ē. Birks	Physics
10.	A. Podelinska	Raman spectroscopy of diamond crystals synthesized by the CVD method	Dr. phys. J. Gabrusenoks	Physics
11.	I. Jansone	The role of multilingual competence in learning English vocabulary	As. Prof. V. Kalnbērziņa	Philology
12.	E. Straumanis	Evaluation and comparison of citation tendencies of scientific articles and their authors	Dr. Phys. A. Zolotarjovs	Computer Science

Other important news in 2021

Achievements

- Ludvigs and Māris Jansons name award in Physics presented by the Latvian Academy of Science received by the leading researcher from the Laboratory of Thin Films **PhD Edgars Butanovs** for his work 'Synthesis and properties of nanowire and transition metal chalcogenide core-shell heterostructures.' Supervisor Dr. Phys. B. Poļakovs.

https://www.lza.lv/images/LM_LZA%20balvas/LZA_balvas_2021/Jansonu%20balva_E.Butanovs_final.pdf

- L'ORÉAL Baltic 'For Women in Science' prize awarded to the scientific assistant of the Laboratory of EXFAS Spectroscopy **Mg. Phys. Inga Pudža** for her work on the research of smart material copper molybdate (CuMoO₄).

<https://www.lza.lv/aktualitates/jaunumi/649-tris-latvijas-zinatnieces-sanem-prestizo-l-oreal-baltic-balvu-sievietem-zinatne>

<https://www.lu.lv/par-mums/lu-mediji/zinas/zina/t/66586/>

<https://labsoflatvia.com/aktuali/2021-sievietem-zinatne>

<https://forbesbaltics.com/lv/zinas/raksts/loreal-baltic-balva-sievietem-zinatne>

<https://unesco.lv/lv/zinatne/tris-latvijas-zinatnieces-sanem-prestizo-loreal-baltic-balvu-sievietem-zinatne/>

- Researcher of the Laboratory of Spectroscopy Dr. phys. Guna Kriekē received the University of Latvia award *Most outstanding doctoral thesis in the fields of nature, medicine, and engineering*. The topic of the dissertation was 'Erbium upconversion luminescence in transparent glass-ceramics containing ternary fluoride nanocrystals.' Supervisor - Dr.Phys. Anatolijs Šarakovskis.

<https://www.lu.lv/zinatne/sasniegumi/atzinibas/>

- **Dr.phys. Roberts Eglītis** was awarded the diploma of the elected true member of the Latvian Academy of Sciences.

<https://www.lza.lv/aktualitates/jaunumi/678-pasniegti-diplomi-2020-gada-ieveletajiem-jaunajiem-akademijas-locekliem>

- Baltic Assembly prize in science was awarded to the ISSP UL's leading researcher **Dr.phys. Roberts Eglītis** for his research cycle 'Theoretical predictions of new materials for energy harvesting and storage.'

<https://www.saeima.lv/lv/aktualitates/saeimas-zinas/30039-baltijas-asamblejas-balvu-zinatne-pasniedz-fizikim-robotam-eglitim>

<https://www.delfi.lv/news/national/politics/foto-baltijas-asamblejas-balvu-zinatne-sanem-fizikis-robotam-eglitim.d?id=53511757>

<https://www.lza.lv/aktualitates/jaunumi/712-baltijas-asamblejas-balvu-zinatne-pasniedz-fizikim-robotam-eglitim>

- Leading researcher from the Laboratory of Spectroscopy **Dr.phys. Vladimirs Pankratovs** was elected a corresponding member of the Latvian Academy of Sciences.

- The Latvian Academy of Sciences named the work explaining the influence of the local atomic structure of molybdates and tungstates on their thermochromic and magnetic properties carried out by

the ISSP UL's researchers **Mg. Phys. Inga Pudža, Dr. rer. nat. Georgijs Bakradze, Dr. Phys. Andris Anspoks, Dr. Phys. Aleksandrs Kaļīnko, and Dr. Phys. Alexei Kuzmin** as the achievement of the year in the field of theoretical science in 2021. <https://www.lsm.lv/raksts/dzive--stils/tehnologijas-un-zinatne/latvijas-petnieku-raditais-pulveris-varetu-noderet-temperaturas-markieriem-vakcinam-un-partikas-produktiem.a438299/>

- The Latvian Academy of Sciences named the work on the development of innovative, high-speed thermoelectric radiation sensor (TESS) carried out by ISSP UL's researchers **Dr. Phys. Mārtiņš Rutkis, Dr. Phys. Kaspars Pudžs, Dr. Phys. Aivars Vembris, and Mg. Phys. Jānis Busenbergs** as the achievement of the year in the field of applied science.

<https://ltv.lsm.lv/lv/raksts/12.01.2022-latvija-rada-inovativu-termo-elektriska-starojuma-sensoru.id249496>

- The Latvian Academy of Sciences Letter of Recognition was awarded to the team of researchers of various institutions involved in the development of the project 'Integration of reliable technologies for protection against Covid-19 in healthcare and high-risk areas' within the National Research Program. Among the authors was the leading researcher of the ISSP UL, head of the Thin Films Laboratory **Dr. habil. Phys. Juris Purāns**.

https://www.lza.lv/images/Sasniegumi/LZA_sasniegumi_atzinibas_2021.pdf

- ISSP UL's Scientific Council voted the leading researcher of the Institute **Dr. Phys. Roberts Rimša** as the ISSP UL's Man of the Year.

Conferences and events organized by the ISSP UL

- February 11-13, the **37th ISSP UL Scientific conference** took place during which 62 oral presentations (three of them were invited speeches) were given. Most of the speakers were students and young scientists.

<https://www.cfi.lu.lv/en/events/conferences/annual-issp-ul-scientific-conference/previous-issp-ul-scientific-conferences/2022/>

- On the last Thursday of almost each month (except for summer and holidays), **ISSP UL' Scientists' Breakfast** takes place online. In 2021, there were 7 events where scientists from the ISSP UL and other scientific institutions talked about their research or important projects and the audience could get involved by asking questions. So, the themes of the Scientists' Breakfast ranged from Latvian scientific expeditions in polar areas, to Ancient Egypt, Latvian efforts in Space research, tropical bug research in Philippines by the Latvian scientists, and many more.

- On April 28, a hybrid **bilateral scientific seminar of the Taiwan and the Baltic States Research Center on Physics** took place. There were 7 speakers and the audience of 30 on-site listeners. 100 people participated in the seminar online.

<https://www.youtube.com/watch?v=s1F-nnngnUo>

- May 13, the annual competition for the school youth "Solar Cup" took place for the 13th time. The competition enabled pupils' (grades 5-12) interest in science and alternative energy sources. 18 teams with the total of 46 participants took part at the online event.

<https://www.cfi.lu.lv/en/events/solar-cup/>

- On November 5-7, student idea marathon – “**Student Deep Science Hackathon**” took place online.

<https://www.camart2.com/en/events/issp-ul-hosts-student-deep-science-hackathon-2021.html>

- December 21 – 22, **IX International Physics Conference in Honor of F. Pianca** jointly organized by the ISSP UL and the Faculty of Physics, Mathematics, and Optometry, University of Latvia took place.
- In 2021 eighteen ISSP UL Doctoral school and other scientific seminars have taken place.

Scientific projects

- In 2021 ISSP UL implemented 76 projects:
 - two Horizon 2020 projects;
 - four COST projects;
 - nineteen ERDF projects;
 - one EAFRD project;
 - four EraNet projects;
 - three *EUROfusion* projects;
 - one Latvia-France bilateral cooperation project OSMOZE;
 - two EEA and Norway cooperation projects;
 - two Latvia-Lithuania-Taiwan Trilateral Scientific Cooperation projects;
 - twenty-three Latvian Council of Science projects;
 - eleven postdoctoral projects;
 - two Latvian Rural Support Service projects;
 - two National Research Program’s projects.

Participation in conferences

- In 2021, ISSP UL researchers participated in more than 18 scientific conferences and seminars. Due to the travel restrictions related to Covid-19, most of the events took place online.
 - February 17-18, representatives from Materize participated in **PHOTONICS+ virtual exhibition and conference**.
 - March 25, ISSP UL’s director Dr. phys. Mārtiņš Rutkis took part in the **27th congress of the Latvian Materials Research Society**.
 - May 9-13, Materize representatives participated in **Compound Semiconductor Week (CSW)**.
 - From May 31 till June 4, researchers from Laboratory of Kinetics in Self-organizing Systems and Laboratory of Spectroscopy took part in virtual spring conference of **European Material Research Society (E-MRS)**.
 - June 7-9, the head of the Laboratory of Thin Films Dr. habil. phys. Juris Purāns participated in **Quantum Complex Matter 2021 Symposium** with the invited speech.
 - July 5-7, ISSP UL young researchers participated in the conference for young researchers **YOUNG MULTIS - Multiscale Phenomena in Condensed Matter**.
 - August 14-22, scientific assistant from the Laboratory of Microscopy Annemarija Trausa participated in **Twenty-Fifth Congress and General Assembly of the International Union of Crystallography**.
 - August 23-27, twelve researchers from the ISSP UL participated in the **23rd international conference-school ADVANCED MATERIALS AND TECHNOLOGIES 2021**.

- September 12-18, **11th International conference LUMDETR** took place. Researchers from Laboratory of Spectroscopy participated in it and leading researcher from Laboratory of Kinetics in Self-organizing Systems Dr. phys. Anatoli Popov presented his report.
- September 24, head of the Laboratory of Computer Modeling of Electronic Structure of Solids Dr. rer. nat. Sergei Piskunov presented his report in the conference **Chemistry and Chemical Technology 2021**.
- From September 28 till October 2, leading researcher from the Laboratory of Thin Films Dr. phys. Vera Skvorcova and leading researcher from Laboratory of Kinetics in Self-organizing Systems Dr. phys. Anatoli Popov (with a report) participated in a conference **OMEE**.
- October 10-14, leading researcher from the Laboratory of Micro and Nanodevices Dr. sc. ing. Roberts Rimša presented his research results at the conference **μTAS 2021**.
- October 13-15, leading researcher from the Laboratory of Spectroscopy Dr. phys. Jurgis Grube participated in conference **OPAL' 2021** with a poster.
- November 22-24, leading researcher from the Laboratory of Computer Modeling of Electronic Structure of Solids Dr. phys. Roberts Eglītis participated at the **ICMSAP-2021 conference** with and invited report.
- November 22-26, representatives from the Laboratory of EXAFS Spectroscopy participated at the conference **IX International Scientific Conference ACTUAL PROBLEMS OF SOLID STATE PHYSICS (APSSP-2021)**.
- November 27-28, young researcher Madara Leimane from the Laboratory of Optical Materials and leading researcher from the Laboratory of Spectroscopy Dr. phys. Anatolijs Šarakovskis took part at the **University of Latvia Student Scientific Conference "Initium"**.
- December 1-3, representatives from Materize participated at the **Optics and Photonics days (OPD 2021)** conference.
- December 12-15, leading researcher from the Laboratory of Micro and Nanodevices Dr. sc. ing. Roberts Rimša with poster presentation participated at the scientific conference **Organoids & Organs-on-Chips 2021**.

Attracting young scientists

• In the regular competition for ISSP UL's Students and Young Scientists grants from Institute's financial reference amount, grants were allocated to the master's degree students **Aija Kalniņa, Haralds Ozols, Miļena Dile**, doctoral students **Andrejs Česnokovs, Kevon Kadiwala Igors Mihailovs, Aleksandrs Platonenko, Edgars Vanags, Jēkabs Cīrulis, Līga Britāla**, and young scientist **Aleksejs Gopejenko**.

Other activities

• On January 25, the Latvian National Television (LTV1) in their morning program **Rīta Panorāmā** broadcasted a story about the most important scientific achievement in theoretical science of the year 2020 voted by the Latvian Academy of Sciences (LAS) – Latvian scientists work on the creation of artificial sun.

https://ltv.lsm.lv/lv/raksts/25.01.2021-latvijas-zinatnieki-strada-pie-maksligas-saules-izveides.id209144/?fbclid=IwAR1KSTvZeUqDVRqfH8aJyTabrE-SjgYfZOm2o_wW4qLqCWRt2KdAtyUZUM

- On January 25, LAS newspaper "**Zinātnes vēstnesis**" (1 (606)) published an article in which ISSP UL's researchers from the Laboratory of Kinetics in Self Organizing systems Dr. phys. Anatoli Popov and Aleksandrs Platoņenko talked about the energy of the future and its relation to the fusion reactor development.

<https://www.lza.lv/aktualitates/jaunumi/418-nakotnes-energetika-ir-saistita-ar-kodolsintezes-reaktoru-attistibu>

- On February 9, a **virtual tour of the ISSP UL** organized by the European Photonics Industry Consortium (EPIC) took place.

<https://www.youtube.com/watch?v=QJVDo6aD3gk&feature=share&fbclid=IwAR0FCRD6RePaKs1jSV5ppxOwD0Q2T4fJeC9tGFg51WeX2l1f1abADQVVkG0>

- On February 11, ISSP UL's Deputy director for innovation Dr. Phys. Andris Anspoks talked to the student radio **NABA** program "**Zinātnes Vārdā**" and explained the audience innovation, Latvian science intensive industry, and deep science.

<https://naba.lsm.lv/lv/raksts/zinatnes-varda/inovacijas-augstas-tehnologijas-latvijas-uznemumos-un-dzila-zina.a140133/>

- On February 16, online platform **Labsoflatvia.lv** published an interview with the ISSP UL researcher and the head of the Communication and Information Department Dr. phys. Līga Grīnberga. In the interview L. Grīnberga talked about the new initiative of the ISSP UL targeted at breaking stereotypes about scientists and giving natural sciences human touch.

https://labsoflatvia.com/aktuali/lauz-stereotipus-par-zinatniekiem?fbclid=IwAR3R9fTxvMZfCXn9JLtltxzWexRQDz5RVRjIM8feD27RpNJ_fhkhVWomaFg

- On February 25, **LTV1** program "**Rīta Panorāma**" broadcasted a story about the innovative methods for improvement of the image quality studied at the ISSP UL.

<https://eng.lsm.lv/article/society/education/latvian-scientists-cleaning-up-image-quality-in-astronomy.a394378/>

<https://baltics.news/2021/02/25/latvian-scientists-are-researching-how-to-improve-image-quality/>

- On February 26, ISSP UL's researchers Dr. Phys. Andris Anspoks and Dr. Phys. Aivars Vembris were guests in the student radio **NABA** program "**Digitālās brokastis**". They tell about the possibilities of development of foldable smart devices.

<https://lr1.lsm.lv/lv/raksts/digitalas-brokastis/viediericu-salokamo-ekranu-attistibas-iespejas.a140731/>

- On March 3, leading researcher from Laboratory of Kinetics in Self-organizing Systems and curator of CERN program Dr. phys. Anatoli Popov participated in a morning program **УТРО НА БАЛТКОМЕ** (Morning on Baltkom Radio) on **Radio Baltkom / Mixnews**.

<https://www.youtube.com/watch?v=-KkNhbjSXbU>

- On March 4, the ISSP UL participated in the **Career Day organized by Riga Technical University** and informed the participants about the career opportunities at the Institute.

- On March 8, leading researcher and head of the Information and Communication department of the ISSP UL Dr. Phys. Līga Grīnberga was a guest at **Radio NABA** program **Studentu pietura** (Student's stop) and told the listeners – how was it to be a woman scientist.

<https://naba.lsm.lv/lv/raksts/studentu-pietura/karjeras-celu-veidojot...-sieviesu-dienas-specializlaidums.a141281/>

- Latvian Public Media (**LSM**) portal published an article by journalist Sandra Kropa-Kaļūznaja “Latvian scientists have discovered the potential for energy production in small coastal waves” in which Dr. phys. Pēteris Lesničenoks talked about his research.

<https://www.lsm.lv/raksts/dzive--stils/vide-un-dzivnieki/latvijas-zinatnieki-atklajusi-energijas-razosanas-potencialu-piekrastes-mazajos-vilnos.a400210/>

- On April 23, morning news program **Rīta Panorāma** of the National Television (LTV1) aired a story about young scientist PhD Edgars Butanovs and his research on nanowires.

<https://ltv.lsm.lv/lv/raksts/23.04.2021-jaunais-zinatnieks-peta-nanovadus.id217753/>

<https://www.lsm.lv/raksts/dzive--stils/tehnologijas-un-zinatne/tukstos-reizu-niecigaki-par-matu-jaunais-zinatnieks-peta-nanovadus.a401728/>

- On April 30, the ISSP UL participated in virtual **European Researchers’ Night**. The aim of the event was to provide an opportunity to get acquainted with the achievements of science and the work of scientists by visiting scientific institutes, universities, and other institutions from all over Latvia.

- On May 13, **magazine Ir** (#19 (575)) published a story about researcher PhD Edgars Butanovs from the Laboratory of Thin Films and his research.

<https://ir.lv/2021/05/12/edgars-butanovs-nanovadu-petnieks/?fbclid=IwAR27vMnWztN5TQ8SeStQ4j5Pp3KO3rNkoSkHCpJQM1ZmclwV0A7jV05x17k>

- On May 27, leading researcher from the Laboratory of Micro and Nano Devices Dr. sc. Ing. Roberts Rimša was a guest in a **Radio NABA program Zinātnes Vārdā** (In the name of science) and talked about his work on organs-on-chips.

<https://naba.lsm.lv/lv/raksts/zinatnes-varda/organs-uz-cipa.a144705/?fbclid=IwAR2nerAp4givuLTz6hsMHQdPhBcz4nBf5FtA2vubZgArgJLBLCDUAZCXp9E>

- On June 8, morning news program **Rīta Panorāma** of the National Television (LTV1) aired a story where leading researcher from the Laboratory of Microscopy Dr. Phys. Krišjānis Šmits talked about nanometer size thin films research.

<https://ltv.lsm.lv/lv/raksts/08.06.2021-iegrave-smilsu-grauda-un-peta-nanometru-planus-slanus.id222169/>

- On June 19, receiver of the L’Oreal Baltic “For Women in Science” award – scientific assistant from the EXAFS Spectroscopy Laboratory Inga Pudža gave an interview on National Radio (**LR 1**).

<https://www.lsm.lv/raksts/dzive--stils/tehnologijas-un-zinatne/ko-spej-sieviete-zinatne-saruna-ar-3-latvijas-zinatniecem.a409726/>

- July 1, receiver of the L’Oreal Baltic “For Women in Science” award Inga Pudža participated in a National Radio (**LR1**) program **Zināmais nezināmajā** (Known in the unknown).

<https://lr1.lsm.lv/lv/raksts/zinamais-nezinamaja/latvijas-zinatnieces-sanem-loreal-baltic-balvu-sievietem-zinatne.a146151/>

- On July 18, portal **labsoflatvia.lv** published an article “Turning a versatile material into a smart thermometer” about the receiver of the L’Oreal Baltic “For Women in Science” award Inga Pudža.

<https://labsoflatvia.com/en/news/turning-a-versatile-material-into-a-smart-thermometer?fbclid=IwAR3ICXIK5BxrFerYD3d-LnznPMnXzZ5JshcEfJUE1-EPvL6VrUOErEwPKjA>

- On July 19, portal **Delfi.lv** published interview with the receivers of the L’Oreal Baltic “For Women in Science” award 2021, including Inga Pudža.

<https://www.delfi.lv/calis/personiba-un-brivais-laiks/stasti-kas-iedvesmo/sievietes-zinatne-solis-cela-uz-vienlidzibu-un-lidztiesibu.d?id=53393893>

- On July 21, University of Latvia Foundation on their website published a story about Inga Pudža, receiver of the L’Oreal Baltic “For Women in Science” award.

<https://www.fonds.lv/par-mums/zinas/zina/t/67055/>

- On July 29, **radio NABA program *Zinātnes vārdā*** (In the name of science) had a guest – ISSP UL’s leading researcher and deputy director for science Dr. habil. phys. Andris Šternbergs. In the program he explained what research Latvian scientists did to secure safe fusion energy for the world in the future.

<https://naba.lsm.lv/lv/raksts/zinatnes-varda/latvija-cela-uz-drosu-kodolenerģiju.-saruna-ar-andri-sternbergu.a147016/>

<https://www.lsm.lv/raksts/dzive--stils/tehnologijas-un-zinatne/fizikis-sternbergs-radit-enerģiju-uz-zemes-ir-izaicinajums.a420085/>

- August 16-17, deputy director for innovation Dr. phys. Andris Anspoks participated in a conference **Skola2030** “LOGOS: Technologies for better education”.

- On August 21, leading researcher from the Laboratory of Micro and Nano Devices Dr. sc. Ing. Roberts Rimša participated in a discussion “Cyber people 2030: cyber-human respect for natural evolution vs. the potential of technology to improve human beings ” at the **Conversation Festival LAMPA**.

- August 26, morning news program **Rīta Panorāma** of the National Television (LTV1) aired a story – portrait of the leading researcher from ISSP UL’s EXAFS Spectroscopy Laboratory Dr. phys. Alexei Kuzmin – Be the First to Discover.

https://replay.lsm.lv/lv/ieraksts/ltv/228925/atklat-pirmajam-pasaule-zinatnieks-aleksejs-kuzmins?fbclid=IwAR0luHegpZC9BBSI3SQU_DQJvjxxh_doaALaQsFGKXHZY8G0ghihrfAKnY

- On August 27-28, deputy director for innovation Dr. phys. Andris Anspoks took part in the **Summer School of the Latvian Association of Young Scientists** “Overcoming the challenges in science”.

- September 10, the **Prime Minister of the Republic of Latvia Krišjānis Kariņš** visited the ISSP UL.

<https://www.mk.gov.lv/lv/jaunums/karins-apmekles-lu-cietvielu-fizikas-institutu>

- On September 21, **ReTV program *Nauda runā*** (Money Talks) was devoted to fight against Covid-19. Among the guests of the program was deputy director for innovation Dr. phys. Andris Anspoks.

<https://www.tvnet.lv/7342191/cina-pret-covid-19-neviens-medikaments-neaizstas-vakcinas>

- On September 23-24, annual event organized by the University of Latvia **Innovation and Tehcnology Day “Knowledge Agora”** took place in which representative of Materize platform and researcher Pēteris Lesničenoks introduced the audience with the innovation opportunities for cooperation with industry offered at ISSP UL.

<https://www.camart2.com/en/events/innovation-opportunities-at-issp-ul-in-cooperation-with-industry.html>

- Latvian Academy of Sciences newspaper **Zinātnes vēstnesis** (Science news) (#8 (613)) in their column “Jubilee Talks” published an interview with the leading researcher from Laboratory of Computer Modeling of Electronic Structure of Solids, academician Roberts Eglītis.

https://www.lza.lv/images/Zinatnes-vestnesis/2021/ZV_09_2021.pdf

- On September 30, leading researcher and head of the Laboratory of Materials for Energy Harvesting and Storage Dr. Phys. Gints Kučinskis was a guest at the National Radio (**LR1**) program **Zināmais Nezināmajā** (Known in the Unknown) where he talked about the batteries of the future.

<https://lr1.lsm.lv/lv/raksts/zinamais-nezinamaja/nakotnes-baterijas-videi-draudzigakas-vai-vieglak-lietojamas.a149635/>

<https://www.lsm.lv/raksts/dzive--stils/vide-un-dzivnieki/bateriju-attistiba-progress-ir-lenaks-neka-to-veletos-skaidro-petnieks-gints-kucinskis.a423801/>

- September 30, **European Hit Radio program Nākotnes formula** (Future Formula) broadcasted a conversation with deputy director for innovation Dr. phys. Andris Anspoks.

<https://www.ehrhiti.lv/podkasti/nakotnes-formula-2021>

- On October 1, National Radio **LR1 program Monopols** (Monopoly) aired an interview with the researcher from the Laboratory of Optical Materials, Doctor of Physics Virgīnija Vītola.

<https://lr1.lsm.lv/lv/raksts/monopols/fizikas-doktore-virginija-vitola.a149550/>

- On October 8, leading researcher from the Laboratory of Ferroelectric Materials Marija Duce participated in an online seminar organized within the scope of **Science.Zoomed.In** events.

- On October 12, researcher from the Laboratory of Optical Materials Dr. Phys. Virgīnija Vītola explained to the listeners of the National Radio (**LR1**) program **Zināmais Nezināmajā** (Known in the Unknown) how the snowflakes were formed.

<https://lr1.lsm.lv/lv/raksts/zinamais-nezinamaja/jaunakie-latvijas-polarpetnieku-atklajumi-par-ledajiem-svalbara.a150170/>

- On October 12, delfi.tv aired a popular science program **Izziņas impulss** (Cognitive Impulse), in which researcher Dr. Phys. Pēteris Lesničenoks talked about on the sustainable future of transport and explained whether we would fill the car tank with hydrogen in the future.

<https://www.delfi.lv/campus/raksti/izzinas-impulss-transporta-ilgtspejiga-nakotne-dizela-vieta-baka-udenradis?id=53645219>

- In October (from 12 till 28), ISSP UL researchers (Baiba Bērziņa, Guna Kriekē; Roberts Rimša; Jānis Kleperis; Pēteris Lesničenoks; Gints Kučinskis; Linards Skuja; Andris Šternbergs; Jurgis Grūbe; Aleksejs Kuzmins; Mārtiņš Rutkis) participated in research project presentation seminars **Tune in to science!** organized by the Latvian Council of Science.

- **Teaming Club meeting** organized by University of Primorska, Slovenia took place on October 20. CAMART² project partners participated in the meeting as well as representatives from Latvia, Estonia, Bulgaria, Cyprus, Czech Republic, Hungary, Poland, Portugal, Serbia, Slovakia, and Slovenia.

<https://www.camart2.com/en/events/online-teaming-club-meeting-2021.html>

- Representatives from Materize platform participated in **EXPO 2020** Dubai on October 22-30.

<https://www.camart2.com/en/events/camart2-team-represents-issp-ul-at-the-expo-2020-dubai-and->

[contacts-potential-collaboration-partners-in-space-industry.html](https://www.camart2.com/en/news/contacts-potential-collaboration-partners-in-space-industry.html)

- October 29, leading researcher from the Laboratory of Visual Perception Dr. phys. Sergejs Fomins was a guest at **Radio NABA program *Digitālās brokastis*** (Digital breakfast) and talked about the parameters of camera development.

<https://lr1.lsm.lv/lv/raksts/digitalas-brokastis/kameru-attistibas-parametri-digitalasbrokastis-intervija.a151170/>

- October 22-25, deputy director for innovation Dr. phys. Andris Anspoks participated at the European Leading 5G ecosystem forum - **5G Techritory**.

<https://www.camart2.com/en/news/director-of-issp-ul-among-the-speakers-at-europes-leading-5g-ecosystem-forum.html>

- October 24-25, deputy director for innovation Dr. phys. Andris Anspoks participated in the **4th Mechanical and Electric Engineering Business Forum**.

<https://www.camart2.com/en/news/director-of-issp-ul-discusses-high-tech-and-innovation-at-the-4th-mechanical-and-electrical-engineering-business-forum.html>

- On November 27, researchers Jānis Teteris and Māra Reinfeldē from the Laboratory of Radiation Physics and expert from the Innovation Department of Materize unit Alfs Raudis presented a series of holographic experiments to schools (3 experiments of different levels of complexity) at the **Physics Teachers' Day** event.

<https://www.camart2.com/en/events/representatives-of-issp-ul-participate-in-physics-teachers-day.html>

- Latvian Academy of Sciences newspaper ***Zinātnes vēstnesis*** (Science news) (#10 (615)) in their column "Jubilee Talks" published an interview with the deputy director for science, academician Andris Šternbergs on November 29.

https://www.lza.lv/images/Zinatnes-vestnesis/2021/ZV_11_2021.pdf

- On December 16, **delfi.lv** published an article "The fusion moment of truth is close. What do Latvians do at the ITER project". In the article the director of the ISSP UL Dr. Phys. Andris Anspoks talked about EUROfusion consortium and how Latvian scientists contributed to the development of fusion.

<https://www.delfi.lv/campus/raksti/kodolsintezes-patiesibas-mirklis-nav-talu-ko-latviesi-dara-gigantiskaja-projekta-iter?id=53872785>

- On December 20, Latvian Academy of Sciences newspaper ***Zinātnes vēstnesis*** (Science news) (#1 (616)) in their column "Jubilee Talks" published an interview with one of the most cited Latvian scientists, leading researcher from the Laboratory of Optical Materials, academician Linards Skuja.

https://www.lza.lv/images/Zinatnes-vestnesis/2021/ZV_12_2021.pdf