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University of Latvia

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Introduction

Institute of Solid State Physics, University of Latvia (ISSP UL) 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 1990ies, after gaining independence and before joining 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 at 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 choose 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 those 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 an 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. 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 – CAMART^2**". 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 the Baltic countries. It was submitted in cooperation with Swedish partners from the Royal Institute of Technology (KTH) and Research Institute of Sweden (RISE). During 12 months of Phase 1, a Business Plan for the future Centre of Excellence CAMART^2 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).

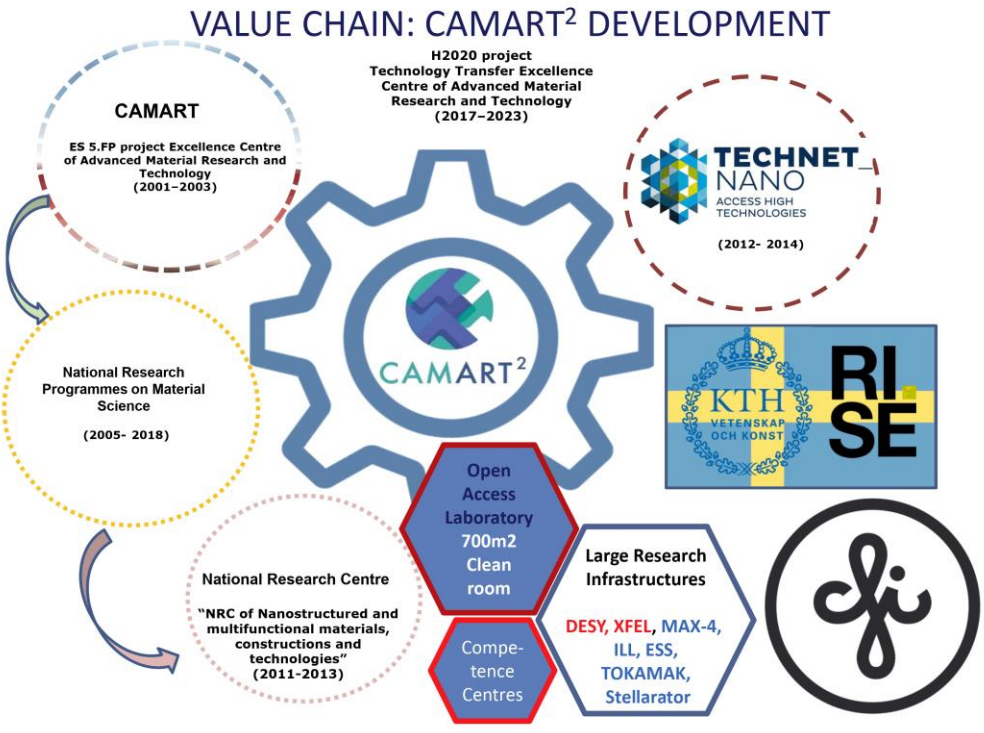


Figure 1: **Value chain: CAMART^2 development.**

ISSP UL has developed strong research and innovation ecosystem.

650 m^2 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's goal is to improve and enhance collaboration with industry in Latvia and abroad. To achieve this, ISSP UL 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 also facilitating communication with companies to carry out projects based on industry-specific standards. Current case studies being undertaken include a cleanroom-based prototyping facility, organic light-emitting diodes, optical lithography, vacuum deposition of thin films and composite nanomaterials synthesis.

Every year "Materize" hosts events for idea creation - Deep Science Hackathons. In February 2020, the 5th Deep Science Hackathon took place with the participation of students and professionals from various Latvia's 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 Research Programme of ISSP UL emphasizes four Priority Directions:

I. Theoretical and experimental studies of materials structure and properties;

II. Nanotechnology, thin films, nanocomposites and ceramics;

III. Functional materials for photonics and electronics;

IV. Materials for energy harvesting and storage.

These Priority research Directions have been strategically established to increase the international visibility of the Institute's scientific capacity and will be further elaborated and implemented within the interdisciplinary cross-laboratory collaboration. The research will be structured towards the application-driven Research & Innovation (R&I) domains where discoveries can make the change thus initiating and establishing the value chain. Realization of Priority Research Directions will be based on the implementation of several measures and activities within Research & Innovation domains.

The Domains system is the basis of the new, advanced project applications development concept, included in the ISSP UL Research Program. It is a novel, well developed and step-by-step system for ensuring the flow of promising project applications.

In the year 2020, the Domain concept continued to show positive results. 67 projects were implemented. They include 2 Horizon 2020, 3 COST projects, 1 European Agricultural Fund for Rural Development (EAFRD) project, 18 European Regional Development Fund projects, 2 EraNet projects, 3 EUROfusion projects, 21 Latvian Council of Science Projects, 10 Postdoctoral projects, 2 Rural support service projects, 1 Latvia - France Bilateral Program “OSMOZE” project, 1 Latvian-Ukrainian Bilateral Cooperation Program in the Area of Science and Technology, 2 Latvia-Lithuania-Taiwan mutual projects and 1 National Research Program.

The structure of ISSP UL at the end of 2020 is as 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 15 members elected by the employees of the Institute (Table 1). Presently, Dr.phys. L.Trinklere 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 2020

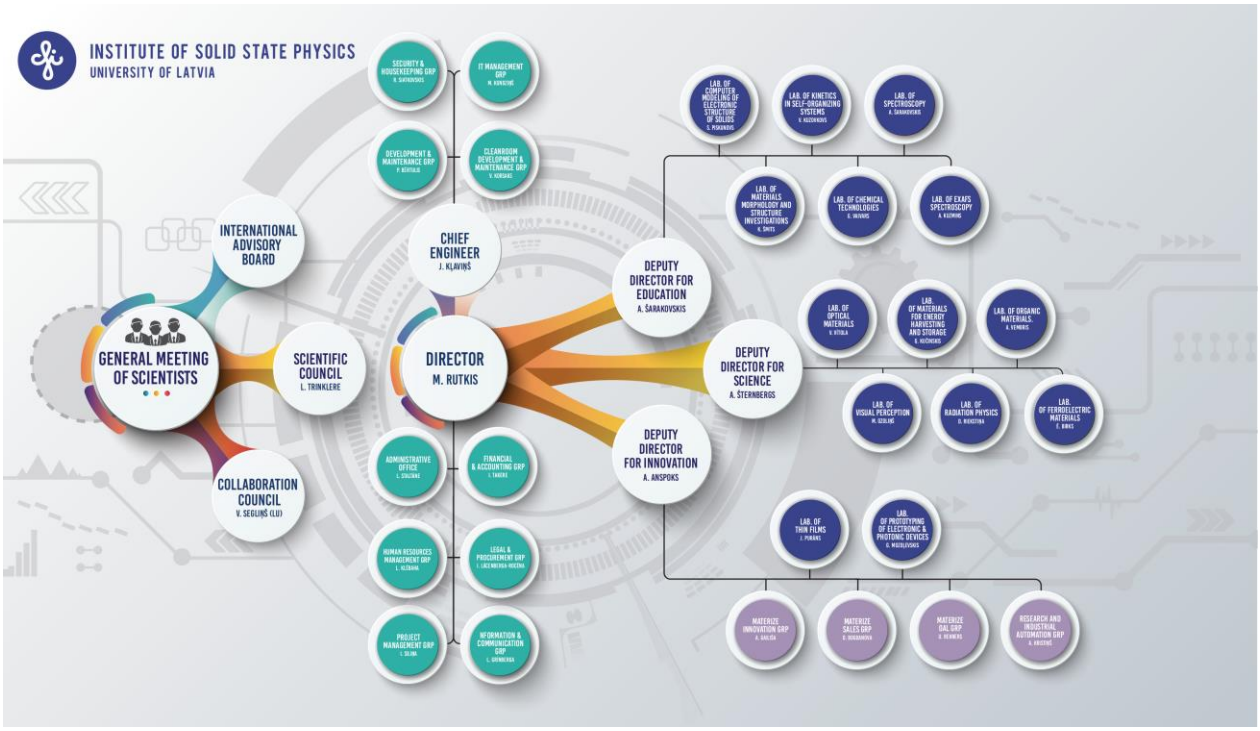


Table 1:

The Scientific Council of the Institute

1. Laima Trinklere, Dr.phys., Chair of the Scientific Council
2. Anatolijs Sarakovskis, Dr.phys., Vice-Chair of the Scientific Council and Deputy Director
3. Andris Anspoks, Dr.phys., Deputy Director
4. Guntars Kitenbergs, Dr.phys., University of Latvia
5. Gunars Bajars, Dr.chem.
6. Dmitrijs Bocarovs, Dr.phys.
7. Liga Grinberga, Dr.phys., Scientific Secretary
8. Janis Kleperis, Dr.phys.
9. Maris Knite, Dr.phys., Riga Technical University
10. Donats Millers, Dr.habil.phys.
11. Martins Rutkis, Dr.phys., Director
12. Andrejs Silins, Dr.habil.phys.
13. Andris Sternbergs, Dr.habil.phys., Deputy director
14. Anatolijs Truhins, Dr.habil.phys.
15. Jurgis Grube, 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 commercialization of scientific results and for improving the management.

Table 2:

The International Advisory Board

1. Prof. Juras Banys, Vilnius University, President of the Lithuanian Academy of Sciences 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
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, DH Consulting at company *Funzionano* , Norway
9. Prof. Marco Kirm, University of Tartu, Estonia
10. Prof. Maija Kuklja, program director at National Science Foundation, USA
11. Dr. Jiri Kulda, scientist emeritus at the 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. Sergei Tuituinnikov, 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 2020, 316 employees were working at the Institute (245 employees at the end of 2019). ISSP UL research staff dynamics is shown in Figure 4, indicating an impressive increase in the number of students involved in the implementation of projects.

This Annual Report summarizes the research activities of the ISSP UL in 2020. 127 papers were published in peer-review journals, 51 of them (40%) in the journals with the SNIP factor >1. The most noticeable achievement during 2020 was a significant increase in the share of publications in the top 10% most cited publications worldwide (Figure 5). Also, despite travel limitations imposed by the COVID-19 pandemic, the ISSP UL researchers were active in disseminating their results at international conferences, most of which were organized as on-line events. More than 60 oral/poster presentations were held at 15 scientific conferences/workshops. The study on "In-depth understanding of the functional properties of modern materials in extreme radiation conditions and their prediction" performed by the ISSP team was recognized by the Latvian Academy of Sciences as one of the ten most significant achievements in Latvian science of in 2020.

Table 3 below summarizes the key performance indicators (KPIs) of ISSP UL. Several positive trends can be easily observed: an increase in the number of publications published in the collaboration with international partners (78%), an increase in the number of citations/year (3186) and the average SNIP per publication (0.948). These numbers indicate positive trends which should be consolidated in subsequent years.

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

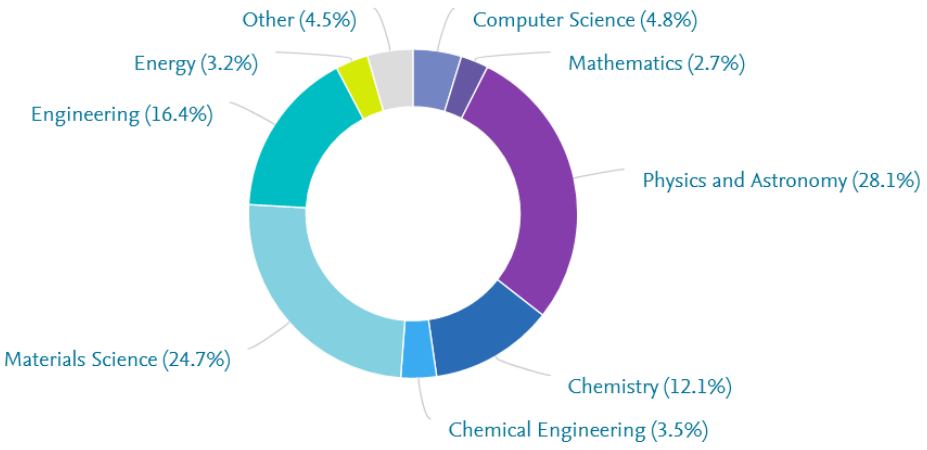


Figure 4: **ISSP UL research staff dynamics 2009-2020**

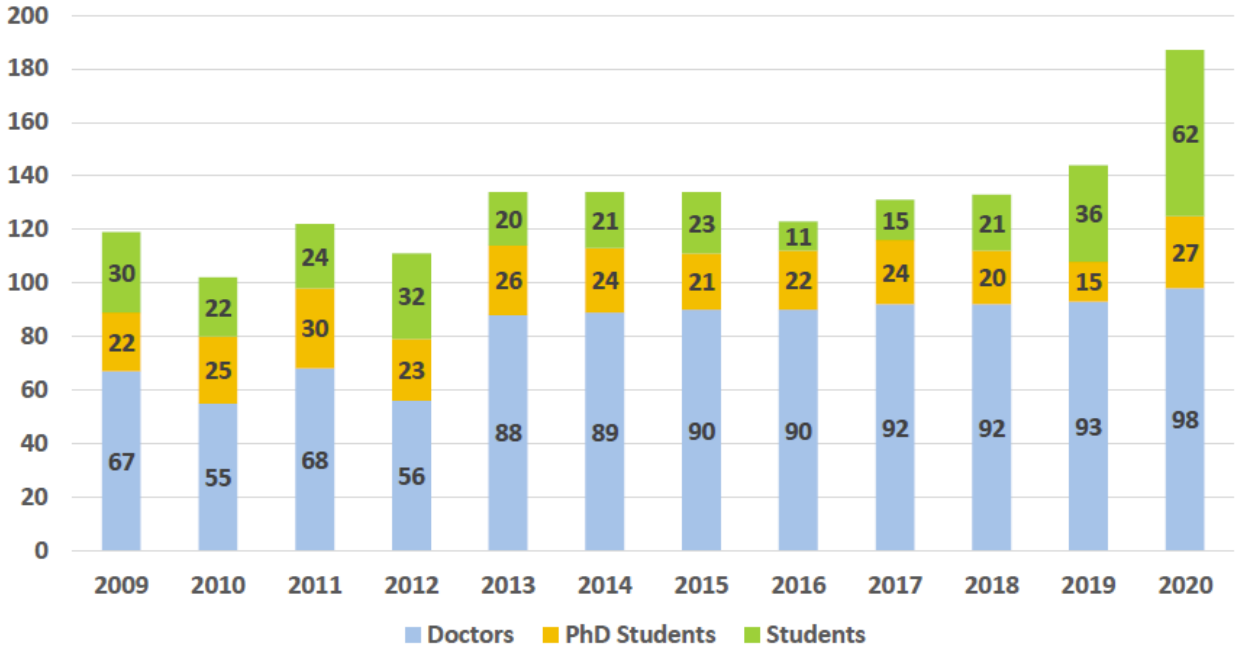


Figure 5: ***Share of publications in ISSP UL in top 10% most cited publications worldwide (from Scopus database)***

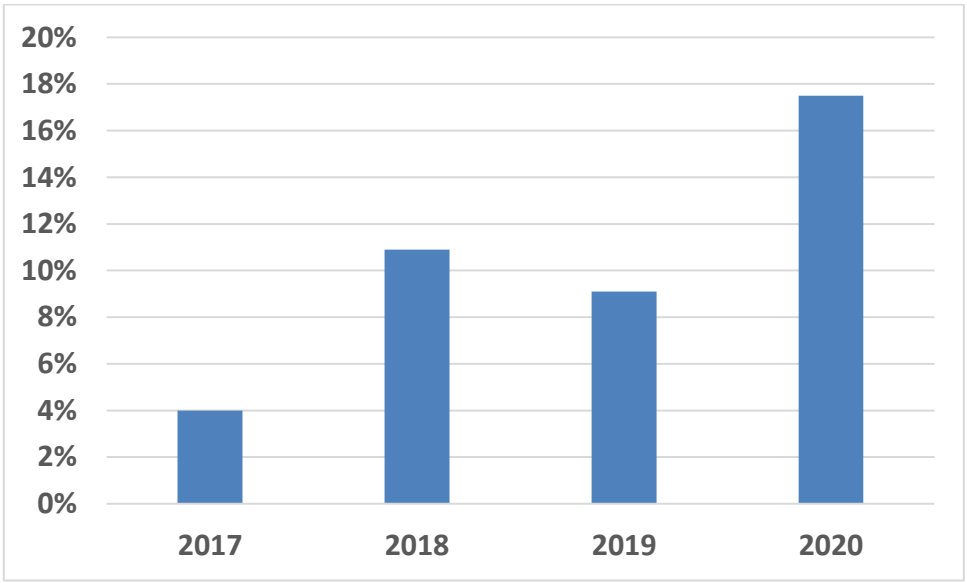


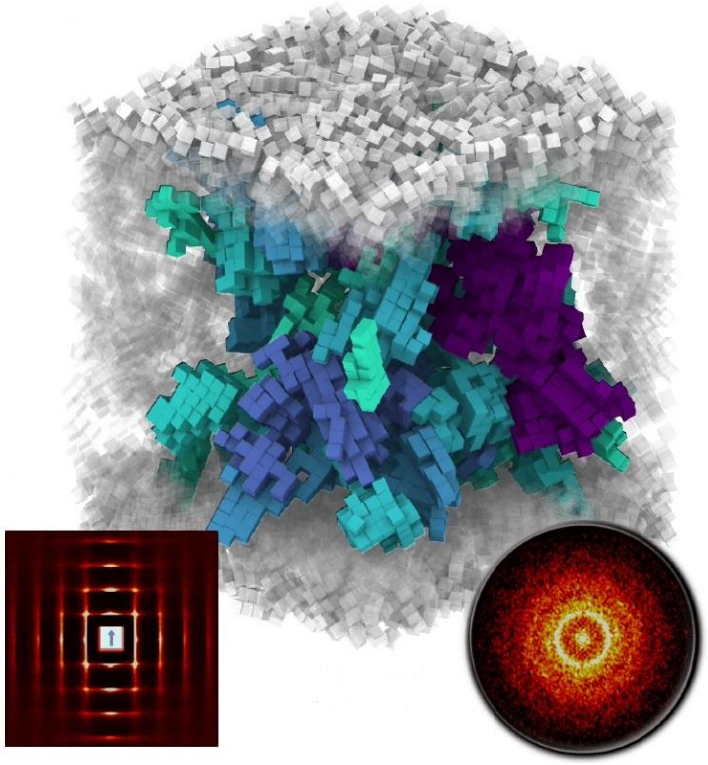
Table 3:

Key performance indicators

Key performance indicators for Research	3 years average (2014-2016)	2017	2018	2019 (Mid-CAMART²)	2020	2023 (End of CAMART²)	2026 (Sustainability)
Number of scientific publications according to "Scopus"	125	100	129	120	**127**	300	400
A fraction of scientific publications in Int. Collaboration (%)	51	61	66	57	**78**	60	65
Number of citations/year according to "Scopus"	2312	2255	2465	2643	**3186**	2 500	5 000
Average SNIP per publications	0.790	0.896	0.875	0.908	**0.948**	1.100	1.250
Number of scientific and technical personnel (FTE)	105	117	126	124	**138**	170	180
Publications/FTE	1.11	0.79	1.02	0.97	**0.92**	1.76	2.22
Gender balance of scientific and technical personnel (% female)	26	22.2	27.2	31	**30**	33	37

Scientific Highlights

I. Theoretical and experimental studies of materials structure and properties.



In-depth understanding of the functional properties of modern materials in extreme radiation conditions and their prediction

A.I. Popov [a], V. Kuzovkov [a], E. Kotomin [a], D. Gryaznov [a], A. Platonenko [a], E. Shablonin [a], A. Lushchik [b]

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It is widely acknowledged that the energy of the future lies in the development of fusion reactors. Their successful work requires new materials that will work in very extreme radiation and temperature conditions. Research on such optical and dielectric materials is an important part of the activities of the EUROfusion-Latvia association. In this joint work of the teams of the Institute of Solid State Physics of the University of Latvia and the Institute of Physics of the University of Tartu, the damage processes caused by neutron and heavy ion irradiation in promising functional materials were investigated. The optical , dielectric as well as vibration and magnetic properties and radiation defects in numerous oxide crystals, nanomaterials and ceramics were carefully studied and compared. Based on this study, we developed new theoretical methods able to evaluate and predict advanced materials functionality and radiation damage evolution under extreme reactor conditions.

Published in

1. *V. Seeman,* ***A. Lushchik, E. Shablonin****, G. Prieditis, D. Gryaznov,* ***A. Platonenko****,* ***E.A. Kotomin****,* ***A.I. Popov,*** *Atomic, electronic and magnetic structure of an oxygen interstitial in neutron-irradiated Al_2O_3 single crystals, Sci. Rep. 10 (2020) 15852, doi:10.1038/s41598-020-72958-9.*
2. ***A. Lushchik,*** *E. Feldbach,* ***E.A. Kotomin****, I. Kudryavtseva,* ***V.N . Kuzovkov****,* ***A.I . Popov****, V. Seeman,* ***E. Shablonin****, Distinctive features of diffusion-controlled radiation defect recombination in stoichiometric magnesium aluminate spinel single crystals and transparent polycrystalline ceramics, Sci. Rep., 10 (2020) 7810, doi:10.1038/s41598-020-64778-8.*
3. ***A. Platonenko****, D. Gryaznov,* ***A.I. Popov****, R. Dovesi,* ***E.A. Kotomin,*** *First principles calculations of the vibrational properties of single and dimer F-type centers in corundum crystals, J. Chem. Phys. 153 (2020) 134107, doi:10.1063/5.0023417.*
4. ***V.N. Kuzovkov****,* ***E.A. Kotomin****,* ***A.I. Popov****, R. Vila, Peculiarities of the diffusion-controlled radiation defect accumulation kinetics under high fluencies, Nucl. Instrum. Methods Phys. Res. B 480 (2020) 45-48, doi:10.1016/j.nimb.2020.07.023.*
5. ***A.I. Popov****, E. Elsts,* ***E.A. Kotomin****, A. Moskina, Z.T. Karipbayev, I. Makarenko, S. Pazylbek,* ***V.N. Kuzovkov****, Thermal annealing of radiation defects in MgF_2 single crystals induced by neutrons at low temperatures, Nucl. Instrum. Methods Phys. Res. B 480 (2020) 16-21, doi:10.1016/j.nimb.2020.07.026.*
6. *G. Baubekova, A. Akilbekov,* ***A.I. Popov****,* ***E. Shablonin****, E. Vasil'chenko, M. Zdorovets,* ***A. Lushchik,*** *About complexity of the 2.16-eV absorption band in MgO crystals irradiated with swift Xe ions, Radiat. Meas. 135 (2020) 106379, doi:10.1016/j.radmeas.2020.106379.*
7. *G. Baubekova, A. Akilbekov,* ***E.A. Kotomin****,* ***V.N. Kuzovkov****,* ***A.I. Popov****,* ***E. Shablonin****, E. Vasil'chenko, M. Zdorovets,* ***A. Lushchik,*** *Thermal annealing of radiation damage produced by swift ^{132}Xe ions in MgO single crystals, Nucl. Instrum. Methods Phys. Res. B 462 (2020) 163-168, doi:10.1016/j.nimb.2019.11.013.*

This work was recognized by the Latvian Academy of Sciences as one of the ten most significant achievements in Latvian science of the year 2020.

Adsorption of rare earth elements onto DNA-functionalized mesoporous carbon

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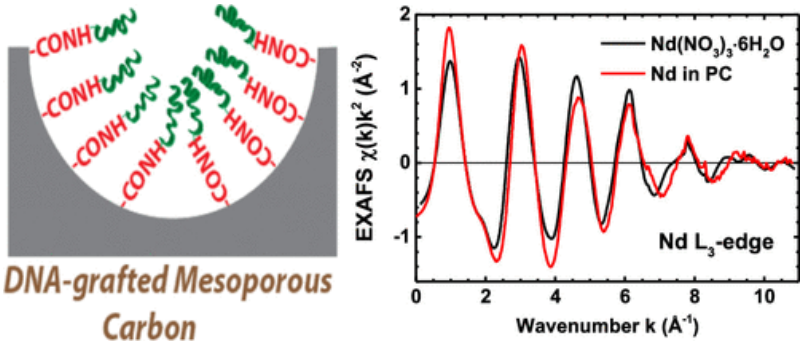
The recovery and separation of rare earth elements (REEs) are of industrial importance owing to the specific usages, high demand, and low supply of these elements. In this study, we have investigated the adsorption of rare earth elements onto DNA-functionalized mesoporous carbons with a BET surface area of 605 m^2/g and a median mesopore width of 48 Å. Three types of single-stranded DNA, one with 100 base units of thymine, another with 20 units of thymine, and the third, a 2000 unit long DNA from salmon milt were grafted on the carboxylated mesoporous carbon surface.

All of the DNA-functionalized mesoporous carbons demonstrated higher adsorption of REEs compared to pristine mesoporous carbon and DNA grafted with 100 units of thymine demonstrated slightly higher adsorbed amounts compared to others. Pure neodymium (Nd(III)) adsorption in the aqueous phase demonstrated an adsorbed amount of 110.4 mg/g with respect to the initial concentration of 500 mg/g. A pH variation study with pure Nd(III) demonstrated that the adsorbed amount is higher at elevated pH compared to that at lower pH, thereby suggesting possible recovery at lower pH. Adsorption of a mixture of 16 REEs, including Sc, Lu, Tm, Yb, Er, Ho, Tb, Dy, Y, Eu, Gd, Sm, Ce, Nd, Pr, and La revealed that the adsorbed amount increased with an increase in the atomic weight and metallic radii of elements within the lanthanides. The calculation of the distribution coefficients for all of the equilibrium adsorption amounts suggested that adsorption is more effective in the lower concentration region. The Nd L_3-edge X-ray absorption near edge structure (XANES) confirmed a 3+ oxidation state of Nd in the adsorbed phase. The extended X-ray absorption fine structure (EXAFS) confirmed the local atomic structure relaxation of Nd complexes in the adsorbed phase and shortening of the Nd−O bond distance by about 0.03−0.04 Å, which may be associated with their local complexation at the carbon surface.



Left panel: Schematic model of DNA-functionalized mesoporous carbon. Right panel: the Nd L_3-edge EXAFS spectra of $Nd(NO_3)_3 \cdot 6H_2O$ and Nd adsorbed onto P- and O-functionalized porous carbon.

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C. E. Unsworth, C. C. Kuo, A. Kuzmin, S. Khalid, D. Saha, ACS Appl. Mater. Interfaces 12 (2020) 43180-43190, doi: 10.1021/acsami.0c09393.

Giant piezoelectricity in B/N doped 4,12,2 – graphyne

D.-C. Yang[a], Z.-W. Tian[b], Y.-K. Chen[a], R.I. Eglitis[c], H.-X. Zhang[a], R. Jia[a]

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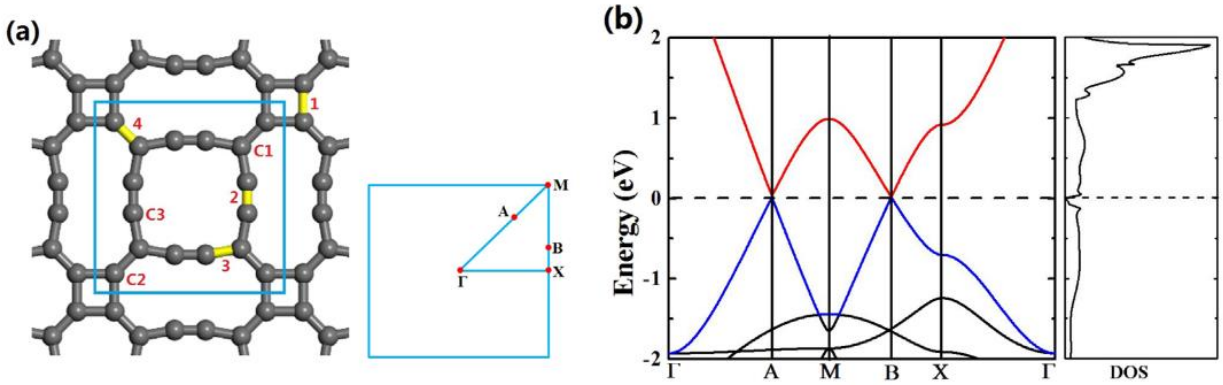
[c]*Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., LV-1063 Riga, Latvia*

The effects of boron (B) and nitrogen (N) substitutions in 4,12,2-graphyne on its geometric structure and mechanical as well as electronic properties have been systematically investigated with the aid of DFT. The trend in the elastic properties of the substituted systems is determined by the doping positions and the type of the dopants. The Bader charge analysis reveals that the N dopant at the sp-site destroys the acetylenic linkage in 4,12,2-graphyne, but instead tends to form a polar bond, or even possibly a charge-shift bond. In particular, an obvious in-plane piezoelectricity is induced by foreign atom substitutions owing to the deformation of the pristine square symmetry.



(a) The sketches for the 4,12,2-graphyne and itsfirst Brillouin zone. The lattice constants area=b= 7.40 Å according to our simulation. The nonequivalentatoms areflagged out. The typical bonds between the carbons are numbered and marked in yellow; (b) The band structure and DOS for the pristine 4,12,2-graphyne.

Published in:
D.-C. Yang, Z.-W. Tian, Y.-K. Chen, R.I. Eglitis, H.-X. Zhang, R. Jia, Applied Surface Science 499 (202) 143800, doi:10.1016/j.apsusc.2019.143800.

Discovery of new boron-rich chalcogenides: orthorhombic B_6X (X=S, Se)

K.A. Cherednichenko[a], V.A. Mukhanov[a], Z. Wang[b,c], A.R. Oganov[b,d,e], A. Kalinko[f,g], I. Dovgaliuk[h], V.L. Solozhenko[a]

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[b] *Skolkovo Institute of Science and Technology, Skolkovo Moscow Region, 143026, Russia*
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[e] *School of Materials Science, Northwestern Polytechnical University, Xi'an, 710072, China*
[f] *Institute of Solid State Physics, University of Latvia, Kengaraga Street 8, LV-1063, Riga, Latvia*
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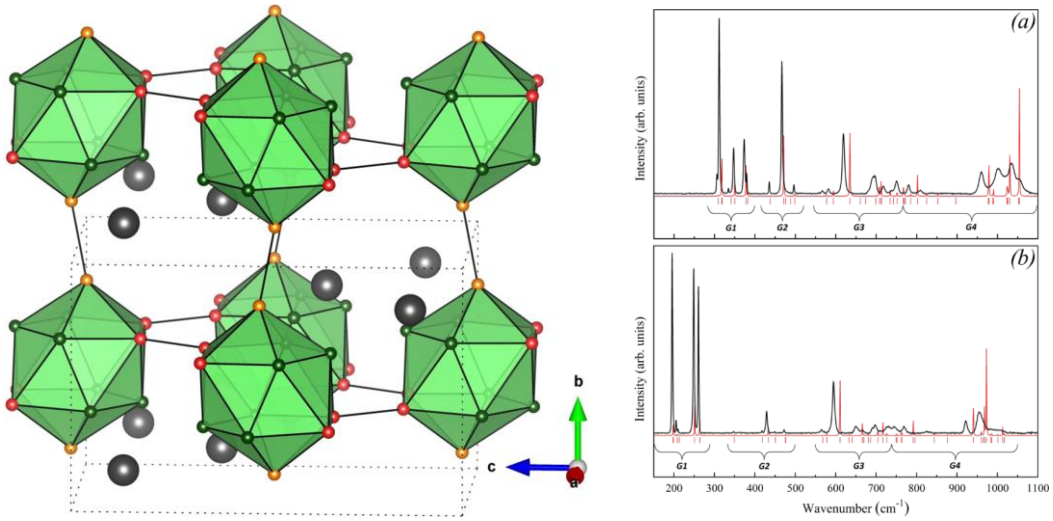
[h] *European Synchrotron Radiation Facility, Grenoble, 38043, France*

New boron-rich sulfide B_6S and selenide B_6Se have been discovered by a combination of high pressure – high-temperature synthesis and ab initio evolutionary crystal structure prediction, and studied by synchrotron X-ray diffraction and Raman spectroscopy at ambient conditions. As it follows from Rietveld refinement of powder X-ray diffraction data, both chalcogenides have orthorhombic symmetry and belong to *Pmna* space group.



Left panel: Crystal structure of new orthorhombic phases of boron-rich sulfide and selenide, o-B_6X (B_{12}-units are presented by green icosahedral polyhedral; polar B1; equatorial B2; and equatorial B3 & B4 atoms are marked by orange, red and green balls, respectively; X = S, Se atoms are shown as large grey balls). *Right panel:* The experimental (black) and calculated by CRYSTAL17 (red) Raman spectra of *o*-B_6S (a) and *o*-B_6Se (b). The red dashes show all predicted Raman active phonon modes.

All experimentally observed Raman bands have been attributed to the theoretically calculated phonon modes, and the mode assignment has been performed. Prediction of mechanical properties (hardness and elastic moduli) of new boron-rich chalcogenides has been made using ab initio calculations, and both compounds were found to be members of a family of hard phases.

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K.A. Cherednichenko, V.A. Mukhanov, Z. Wang, A.R. Oganov, A. Kalinko, I. Dovgaliuk, V.L. Solozhenko, Sci. Rep. 10 (2020) 9277, doi:10.1038/s41598-020-66316-y.

2D slab models of TiO_2 nanotubes for simulation of water adsorption: Validation over a diameter range

O. Lisovski[a,b], S. Piskunov[a], D. Bocharov[a,c], S. Kenmoe[b]

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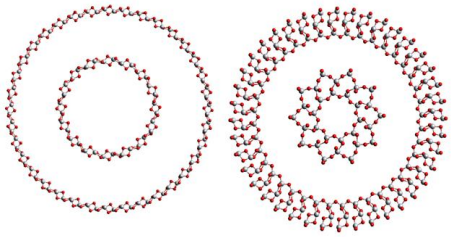
[c] *Transport and Telecommunication Institute, Riga LV-1019, Latvia*

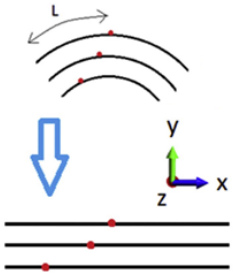
Low-dimensional structures (i.e., structures with one dimension significantly larger than the other two), such as nanorods and nanotubes, are considered to be prospective materials in many applications, for example, photocatalysis and hydrogen generation. The advantage of nanotubes is thin walls, which ensures shorter charge transfer paths and better charge separation, and, consequently, higher process efficiency, which is needed for the technology commercialization.



Examples of TiO_2 nanotubes (cross-section).

Regardless of the fact that nanotubes can be synthesized and are studied experimentally, the amount of papers on computer simulation of nanotubes is not abundant. The reason is that calculations of realistic size nanotube models, especially with water molecules, are very costly in terms of computational power, and will remain so in the nearest future.

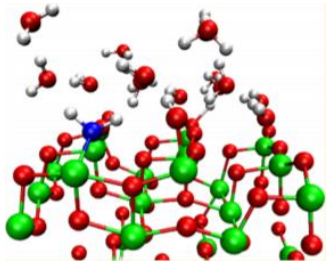
In turn, simulation of such models is required for a better understanding of water photocatalytic splitting processes. There is a typical approach for this problem: a 2D periodic structure, or slab, is used as a nanotube surface approximation. In this way, it is possible to use system translation symmetry and reduce the required computational power. While this approach ensures sufficient precision for large nanotubes (since their curvature is not so prominent, and their properties are closer to a slab), it does not provide adequate precision for small and medium diameters.



Translation of nanotubular atomic coordinates (1D-periodic) into 2D-periodic structure.

Therefore, there is a necessity for a method, which would enable researchers to simulate water adsorption on different nanotubes, preserving their properties.

Within the current study a method of nanotube simulation via modified 2D-periodic structures with partial geometry preservation, elaborated by our group previously, was validated for a large range of nanotube diameters, thus proving systematic performance. One more outcome of the study is a prediction that the method is universal and usable not only for TiO_2, but also for other nanotubes, and for other molecule adsorption simulation.



2D structure with nanotubular geometry motifs, which ensures simulation of water adsorption on nanotube surface.

Published:
O. Lisovski, S. Piskunov, D. Bocharov, S. Kenmoe, Results in Physics 19 (2020) 103527, doi:10.1016/j.rinp.2020.103527.

Co-doping with boron and nitrogen Impurities in T-carbon

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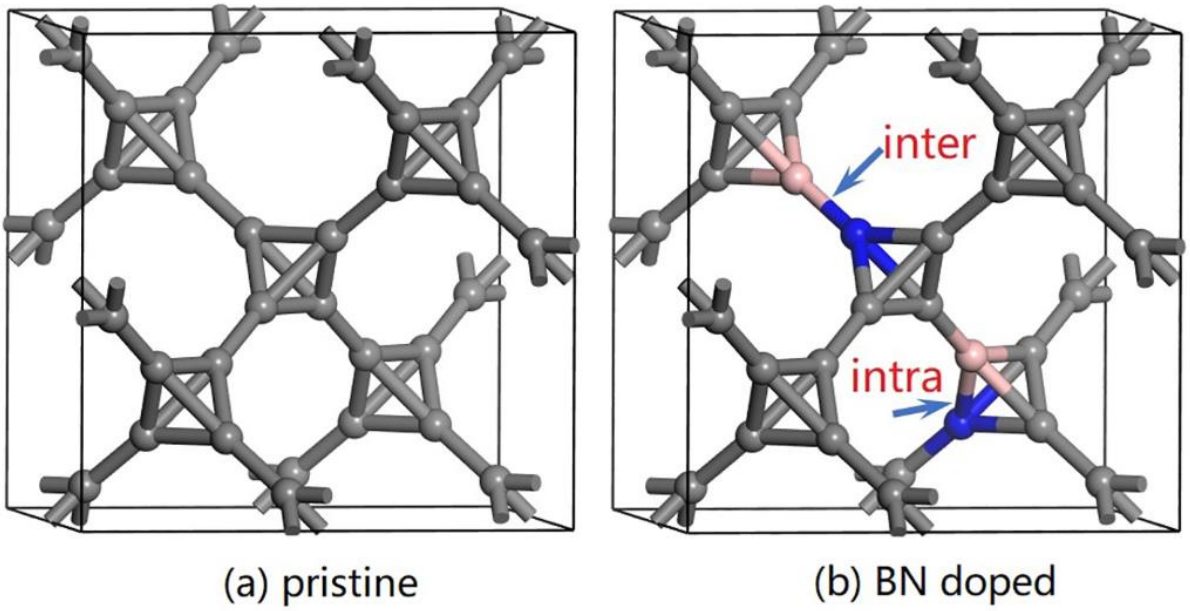
Previously, Ren et al. [Chem. Phys. 518, 69-73 (2019)] reported the failure of Boron-Nitrogen (B-N) co-doping as inter B-N bond in T-carbon. In the present work, a B-N atom pair is introduced in T-carbon as p-n co-dopant to substitute two carbon atoms in the same carbon tetrahedron and form an intra B-N bond. The stability of this doping system is verified from energy, lattice dynamic, and thermodynamic aspects. According to our B3PW calculations, B-N impurities in this situation can reduce the band gap of T-carbon from 2.95 eV to 2.55 eV, making this material a promising photocatalyst.



(a) Atomic configurations for pristine T-carbon, and (b) the sketch of the B-N doping positions in T-carbon. Note that the geometric configurations will be totally changed after B-N co-doping, including the space group, the lattice parameters, and the bonds. Here, we illustrate the atomic sketch of the doping system before the geometry relaxations to clearly show the different doping arrangements. Note that the gray, blue, and pink spheres are represented for carbon, nitrogen, and boron atoms, respectively.

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Z.W. Tian, X.Q. Cui, J.K. Tian, M.C. Cui, L. Jin, R. Jia, R.I. Eglitis, J. Saudi Chem. Soc. 24 (2020) 857-864, doi:10.1016/j.jscs.2020.09.002.

A novel T-C_3N and seawater desalination

J.Q. Zhou[a], L. Li[a], C. Fu[b,c], J. Wang[a], P. Fu[a,d], C.P. Kong[a], F.Q. Bai[a], R.I. Eglitis[d], H.X. Zhang[a], R. Jia[a,d]

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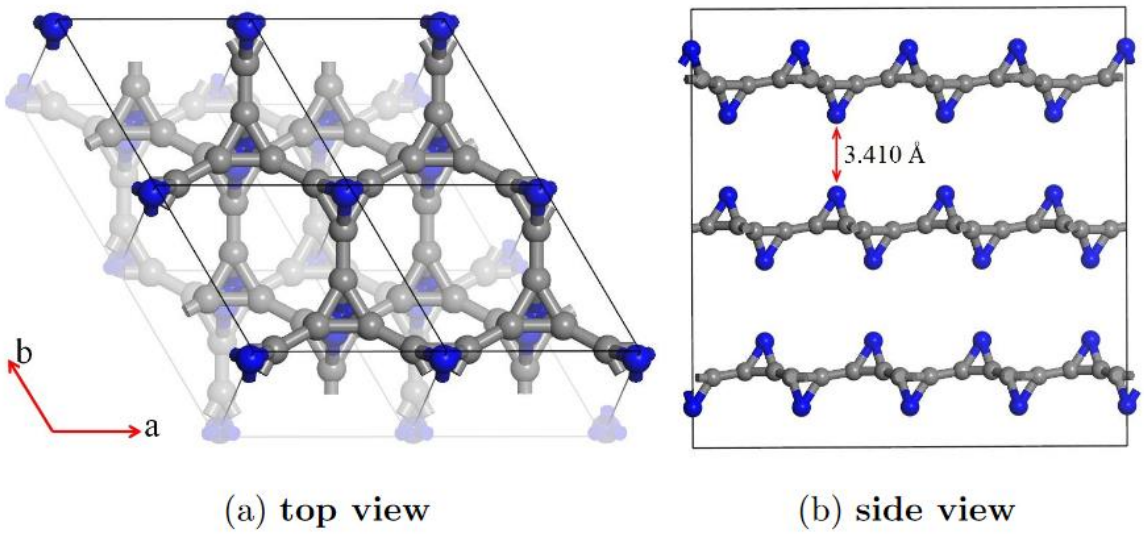
A structurally stable stacked multilayer carbonitride is predicted with the aid of ab initio calculations. This carbonitride consists of C_3N tetrahedral, and is similar to T-carbon and thus named T-C_3N. Its 2-dimensional monolayer is also carefully investigated in this work. The studies on electronic properties reveal that bulk and 2D T-C_3N are insulators with a 5.542 eV indirect band gap and a 5.741 eV direct band gap. However, the monolayer T-C_3N exhibits an excellent uniform porosity. Its 5.50 Å pore size is perfect for water nanofiltration. The adsorption and permeation of water molecules on the monolayer T-C_3N are investigated. Its promising potential application in highly efficient nanofiltration membranes for seawater desalination is discussed.



Sketches for top (a) and side (b) views of a 3D T-C3N in ABCstacking form.

Published in:
J.Q. Zhou, L. Li, C. Fu, J. Wang, P. Fu, C.P. Kong, F.Q. Bai, R.I. Eglitis, H.X. Zhang, R. Jia, Nanoscale 12 (2020) 5055-5066, doi:10.1039/C9NR08108A.

Treatment of disorder effects in X-ray absorption spectra beyond the conventional approach

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[b] *International Research Organization for Advanced Science and Technology (IROAST), Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto 860-8555, Japan*
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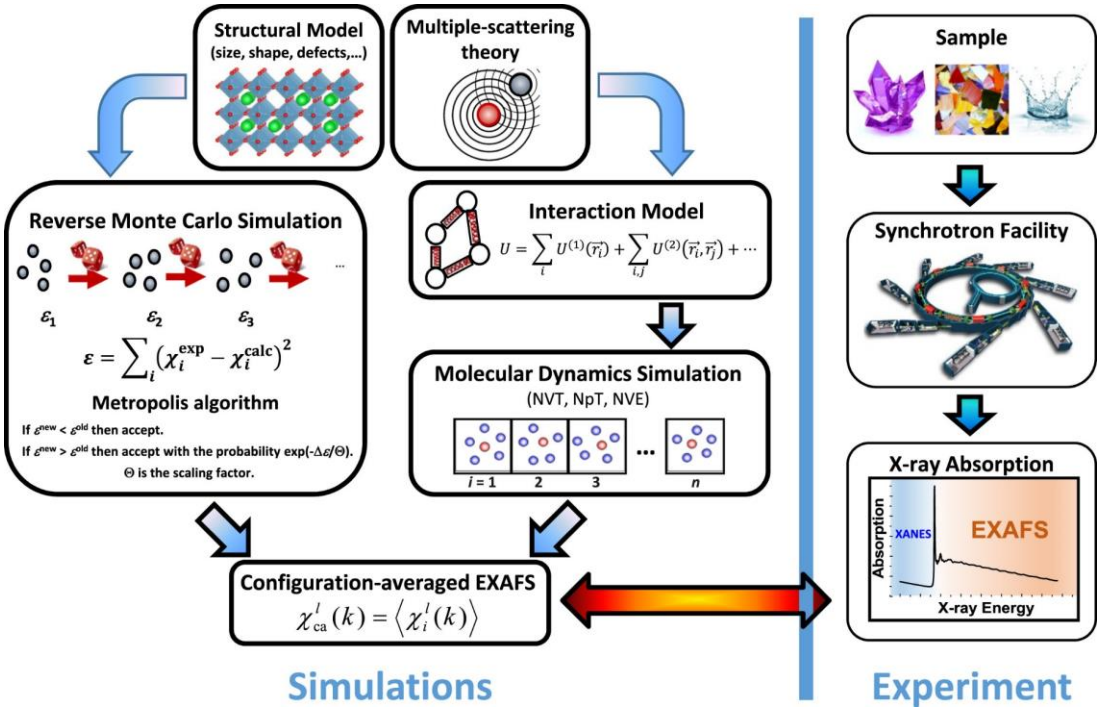
[b] *Universität Paderborn, Naturwissenschaftliche Fakultät, Department Chemie, Warburger Straße 100, 33098, Paderborn, Germany*

The contribution of the static and thermal disorder is one of the largest challenges for the accurate determination of the atomic structure from the extended X-ray absorption fine structure (EXAFS). Although there are several generally accepted approaches to solve this problem, which are widely used in the EXAFS data analysis, they often provide less accurate results when applied to outer coordination shells around the absorbing atom. In this case, the advanced techniques based on the molecular dynamics and reverse Monte Carlo simulations are known to be more appropriate: their strengths and weaknesses are reviewed in this work.



Scheme of EXAFS analysis using reverse Monte Carlo and molecular dynamics methods.

Published in:
A.Kuzmin, J. Timoshenko, A. Kalinko, I. Jonane, A. Anspoks, Rad. Phys. Chem. 175 (2020) 108112, doi:10.1016/j.radphyschem.2018.12.032.

Interpretation of the Cu K-edge EXAFS spectra of Cu_3N using ab initio molecular dynamics

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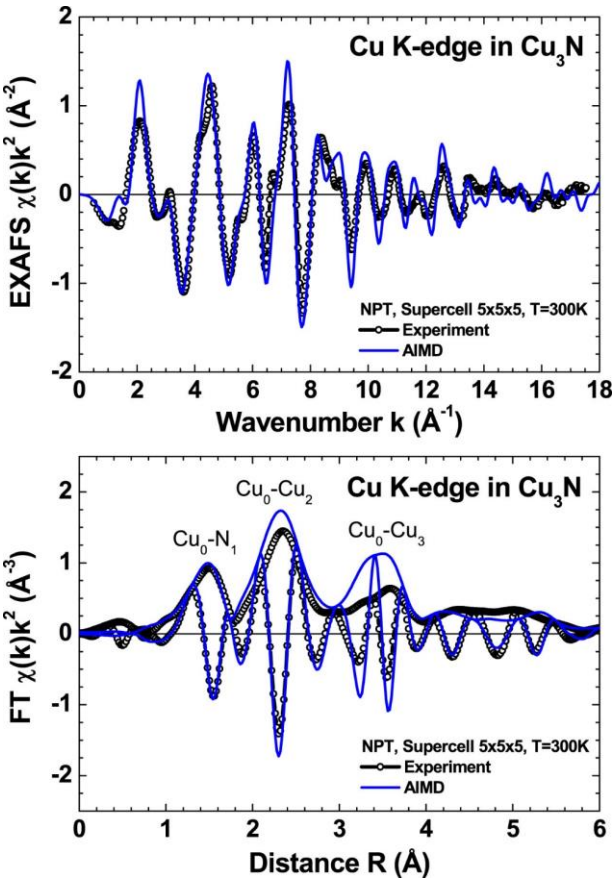
Cubic copper nitride (Cu_3N) has anti-perovskite structure composed of the NCu_6 octahedra joined by corners, and its properties are strongly affected by anisotropic thermal vibrations of copper atoms, having larger amplitude orthogonal to linear –N–Cu–N– atomic chains. Cu_3N is a potentially interesting candidate for many applications such as write-once read-many (WORM) optical storage devices, non-volatile magnetic random access memories and optical lithography for the fabrication of microscopic metal links. Electro-catalytic properties of copper nitride in alkaline fuel cells were also reported, and its usage as an absorber for photovoltaic and photo-electrochemical solar cells was recently demonstrated.

Ab initio molecular dynamics (AIMD) simulations of cubic Cu_3N were performed within the NpT ensemble in the temperature range between 300 and 700 K. The AIMD results were validated using the MD-EXAFS approach by direct comparison with the Cu K-edge EXAFS of polycrystalline Cu_3N at 300 K. The simulations predict strong anharmonicity of Cu–N and Cu–Cu bonds, the anisotropy of Cu atoms vibrations, the rigidity of NCu_6 octahedra and strong correlation in atomic motion within –N–Cu–N– atom chains. These findings are in agreement with our previous reverse Monte Carlo analysis of low-temperature (10–300 K) EXAFS data.



The experimental and AIMD calculated Cu K-edge EXAFS spectra (top panel) and their Fourier transforms (FTs) (bottom panel) at 300 K.

Published in:
D. Bocharov, A. Anspoks, J. Timoshenko, A. Kalinko, M. Krack, A. Kuzmin, Rad. Phys. Chem. 175 (2020) 108100, doi:10.1016/j.radphyschem.2018.12.020.

Local structure of A-atom in ABO_3 perovskites studies by RMC-EXAFS

A. Anspoks[a], C. Marini[b], T. Miyanaga[c], B. Joseph[d], A. Kuzmin[a], J. Purans[a], J. Timoshenko[e], A. Bussmann-Holder[f]

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[b] ALBA Synchrotron Light Source, Crta. BP 1413, Km. 3.3, 08290 Cerdanyola Del Vallès, Barcelona, Spain
[c] *Hirosaki University, Japan*
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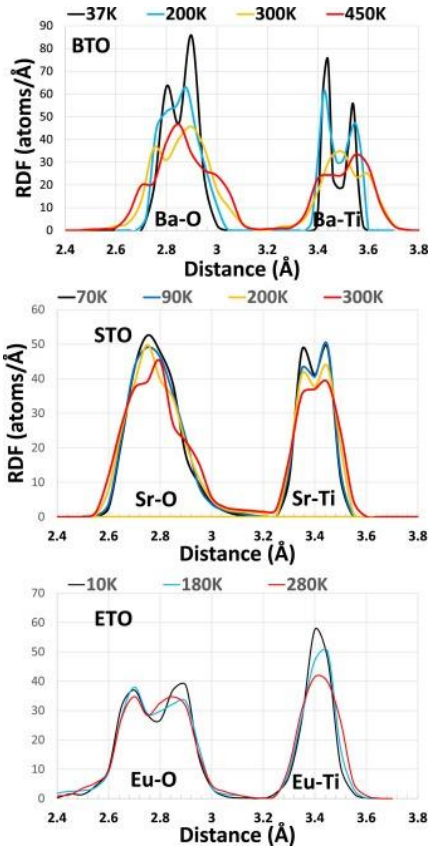
The ferroelectric distortions in perovskites were a subject of numerous investigations for a long time. However, some controversial results still exist, coming from the analysis of diffraction (X-ray, neutron or electron) data and X-ray absorption spectra. In this study, our goal was to revisit these classical materials using recently developed methods without imposing any predefined structural model. Local environment around A-type atom in ABO_3 perovskites ($SrTiO_3$, $BaTiO_3$, $EuTiO_3$) was studied by X-ray absorption spectroscopy (XAS) in a wide range of temperatures (20–400 K). Using the reverse Monte Carlo method enhanced by an evolutionary algorithm, the 3D structure was extracted from the extended X-ray absorption fine structure (EXAFS) and interpreted in terms of the radial distribution functions (RDFs). Our findings show that both diffraction and XAS data are consistent, but reflect the structure of the material from different points of view. In particular, when strong correlations in the motion of certain atoms are present, the information obtained by XAS might lead to a different from the expected shape of the RDF. At the same time, the average positions of all atoms are in good agreement with those given by diffraction. This makes XAS an important technique for studying interatomic correlations and lattice dynamics.



Radial distribution functions (RDF) for Ba–O, Ba–Ti, Sr–O, Sr–Ti, Eu–O, Eu–Ti at different temperatures obtained from $BaTiO_3$, $SrTiO_3$, $EuTiO_3$ EXAFS spectra using our RMC/EA-EXAFS analysis.

Published in:
A. Anspoks, C. Marini, T. Miyanaga, B. Joseph, A. Kuzmin, J. Purans, J. Timoshenko, A. Bussmann-Holder, Rad. Phys. Chem. 175 (2020) 108072, doi:10.1016/j.radphyschem.2018.11.026.

Ab initio molecular dynamics simulations of negative thermal expansion in ScF_3: the effect of the supercell size

D. Bocharov[a], M. Krack[b], Yu. Rafalskij[a], A. Kuzmin[a], J. Purans[a]

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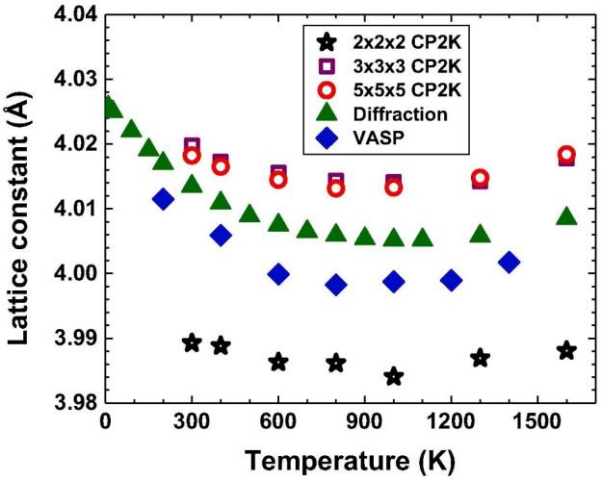
Materials with negative thermal expansion (NTE), contracting upon heating, are not only of great interest from a fundamental physics point of view, but have also high industrial importance. Composites containing NTE components can possess zero thermal expansion, making them suitable for high-precision devices, like space telescope mirrors, teeth fillings, substrates in microelectronics, fuel cells, thermoelectric converters and for many other applications

Scandium fluoride (ScF_3) belongs to a class of negative thermal expansion (NTE) materials. It shows a strong lattice contraction up to about 1000 K switching to expansion at higher temperatures. The ab initio molecular dynamics (AIMD) simulations performed within the isothermal-isobaric (NpT) ensemble as presented in this study can reproduce the negative thermal expansion of ScF_3 up to 1000 K and the positive expansion at higher temperatures in agreement with previous diffraction data. The origin of the NTE in ScF_3 is explained by the interplay between expansion and rotation of ScF_6 octahedra.



Comparison of the temperature dependences of the lattice constant of ScF_3 calculated in this work for 2a × 2a × 2a (open asterisks), 3a × 3a × 3a (open squares), 5a × 5a × 5a (open circles) supercell using CP2K code, calculated for 2a × 2a × 2a supercell by VASP code (solid diamonds) and experimental data (solid triangles).

At the same time, the simulations based on the smallest supercell ($2a \times 2a \times 2a$) fail to describe thermal disorder accurately, leading to an overestimated broadening of the inter-octahedral Sc–F–Sc bond angle distribution and of the outer coordination shells (starting from the third) in the radial distribution functions of scandium.

The results obtained by the AIMD simulations were validated using the MD-EXAFS approach based on the ab initio multiple-scattering theory. A comparison between the calculated and experimental Sc K-edge EXAFS spectra at T=600 K suggests that a supercell larger than $2a \times 2a \times 2a$ should be employed to obtain good agreement, and the best results are achieved for a supercell of at least $4a \times 4a \times 4a$. Thus, we demonstrated that the results of the AIMD simulations are sensitive to the size of the supercell, and the experimental EXAFS spectra can be used to distinguish between different theoretical models.

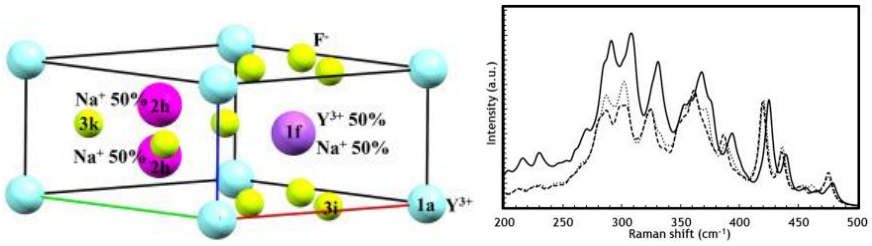
Published in:
D. Bocharov, M. Krack, Yu. Rafalskij, A. Kuzmin, J. Purans, Comp. Mater. Sci. 171 (2020) 109198, doi:10.1016/j.commatsci.2019.109198.

Structural and electronic properties of β-$NaYF_4$ and β-$NaYF_4$:Ce^{3+}

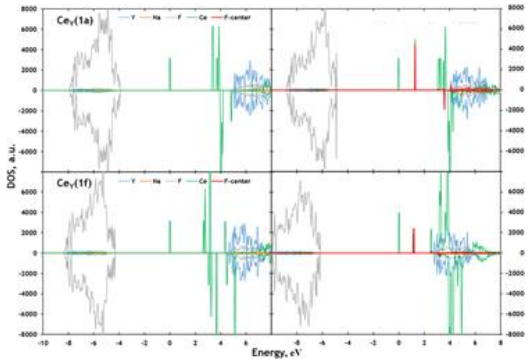
A. Platonenko and A. I. Popov

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

In the present paper, we performed the state-of-the-art ab initio electronic and atomic structure calculations for pure and Ce-doped $NaYF_4$ crystals, which is known to demonstrate excellent luminescence properties. In particular, the density functional theory approach with linear combination of atomic orbitals (LCAO) as implemented in the CRYSTAL17 computer code is applied to hexagonal β-$NaYF_4$, located in three possible space groups of this compound, P6, P63/m and P6 2 m. First, the disordered crystalline structure of $NaYF_4$ was modelled in a large supercell containing 108 atoms. In order to obtain better agreement with the experimental data, we used several different exchange-correlation functionals. Basic properties, such as lattice constant, band gap and total energies were calculated and compared for all three space groups and three exchange-correlation functionals - HSE06, PWGGA and PWGGA+13%HF. It was found that for all three functionals, the minimum of total energy corresponds to space group. Secondly, in order to study the effects associated with the Ce^{3+} impurity and the *F* center (radiation defect), the β-$NaYF_4$ structure with the *F* center and Ce^{3+} or with both was carefully modelled. Taking into account that fluorine atoms have different nearest neighbours, several types of fluorine vacancies were simulated and an appropriate formation energies were determined. Finally, the effects of Ce^{3+} ion substitution of Y ions in different positions as well as formation of Ce^{3+}, the *F* center defect pairs were also studied and an appropriate incorporation energies were calculated.



Crystal structure of β-$NaYF_4$ and calculated Raman spectra for three space groups: P6 (solid line), P6 2 m (dotted line) and $P6_{3/m}$ (dashed line).



Partial Density of States of Ce^{3+} doped $NaYF_4$. Top figures correspond to Ce_Y substitution on 1a position, bottom figure - Ce_Y on 1f position. The positive and negative parts represent the spin-up and spin-down states, respectively. The F-center and Ce^{3+} DOS are multiplied 20x. Zero energy corresponds to highest occupied energy level of Ce^{3+} ion. F-centers produce one additional occupied level above the energy level of Ce^{3+} ion.

Published in:
A. Platonenko and A. I. Popov, Optical Materials 99 (2020) 109529, doi:10.1016/j.optmat.2019.109529.

Origin of pressure-induced insulator-to-metal transition in the van der Waals compounds $FePS_3$ and $FePSe_3$ from first-principles calculations

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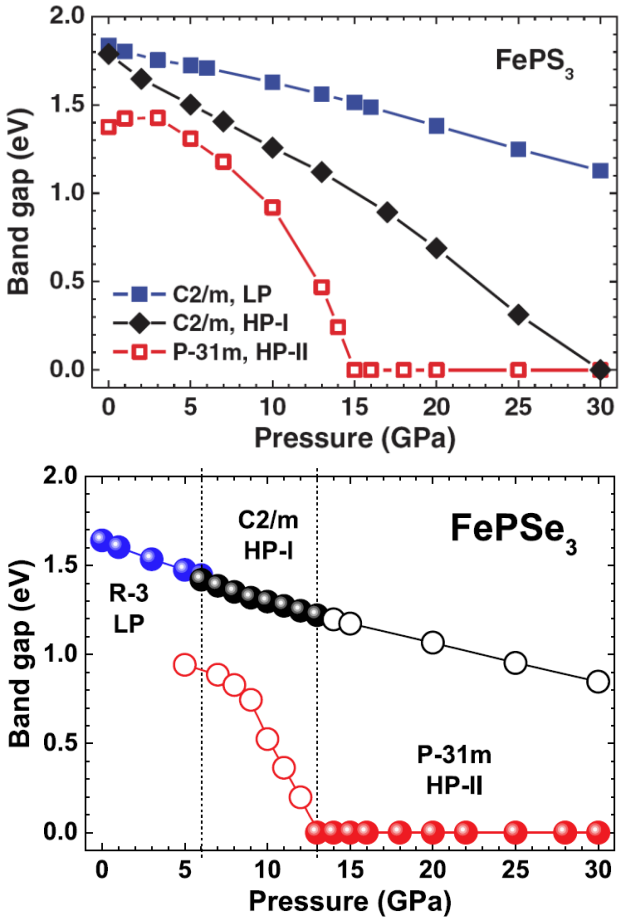
Pressure-induced insulator-to-metal transition (IMT) has been studied in the van der Waals (vdW) compounds iron thiophosphate ($FePS_3$) and iron phosphorus triselenide ($FePSe_3$) using first-principles calculations within the periodic linear combination of atomic orbitals method with hybrid Hartree-Fock-DFT B3LYP functional. Our calculations reproduce correctly the IMTs at about 15 GPa in $FePS_3$ and about 13 GPa in $FePSe_3$. Both transitions are accompanied by a reduction of the unit cell volume and the vdW gap. We found from the detailed analysis of the projected density of states that the 3p states of phosphorus atoms contribute significantly at the bottom of the conduction band. As a result, the collapse of the band gap occurs due to changes in the electronic structure of $FePS(Se)_3$ induced by relative displacements of phosphorus or sulfur/selenium atoms along the c-axis direction under pressure.

The results of the topological analysis of the electron density and its Laplacian in $FePSe_3$ demonstrated that the pressure changes not only the interatomic distances but also the bond nature between the intralayer and interlayer phosphorus atoms. The interlayer P–P interactions are absent in two non-metallic $FePSe_3$ phases, while after IMT the intralayer P–P interactions weaken and the interlayer P–P interactions appear.



Pressure dependence of the calculated band gap in $FePS_3$ and $FePSe_3$.

Published in:
R. A. Evarestov and A. Kuzmin, J. Comput. Chem. 41 (2020) 1337-1344, doi:10.1002/jcc.26178 & J. Comput. Chem. 41 (2020) 2610-2623, doi:10.1002/jcc.26416.

Ab initio calculations of $CaZrO_3$ (011) surfaces: systematic trends in polar (011) surface calculations of ABO_3 perovskites

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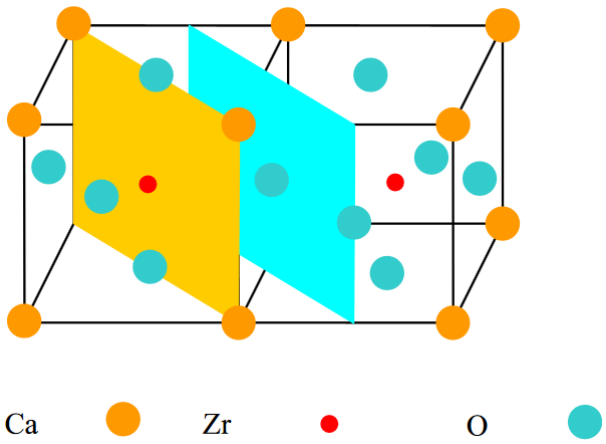
[2]*Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, 130023 Changchun, PR China*

Using the CRYSTAL computer program package, first principles calculations of polar ZrO, Ca and O-terminated $CaZrO_3$ (011) surfaces were performed. Our calculation results for polar $CaZrO_3$ (011) surfaces are compared with the previous *ab initio* calculation results for ABO_3 perovskite (011) and (001) surfaces. As follows from the results of our hybrid B3LYP calculations, all upper layer atoms on the ZrO, Ca and O-terminated $CaZrO_3$ (011) surfaces relax inwards. The only exception from this systematic trend is the outward relaxation of the oxygen atom on the ZrO-terminated $CaZrO_3$ (011) surface. Different ZrO, Ca and O-terminations of the $CaZrO_3$ (011) surface lead to a quite different surface energy of 3.46, 1.49, and 2.08 eV. Our calculations predict a considerable increase in the Zr-O chemical bond covalency near the $CaZrO_3$ (011) surface, both in the directions perpendicular to the surface (0.240*e*) as well as in the plane (0.138*e*), as compared to the $CaZrO_3$ (001) surface (0.102*e*) and to the bulk (0.086*e*). Such increase in the B-O chemical bond population from the bulk towards the (001) and especially (011) surfaces is a systematic trend in all eight our calculated ABO_3 perovskites.



Schematic picture of the cubic $CaZrO_3$ perovskite structure containing two (011) cleavage planes which create charged O_2 and CaZrO (011) surfaces.

Published in:
R.I. Eglitis, J. Kleperis, J. Purans, A.I. Popov, R. Jia, J. Mater. Sci. 55 (2020) 203-217, doi:10.1007/s10853-019-04016-3.

Dynamics of singlet oxygen molecule trapped in silica glass studied by luminescence polarization anisotropy and density functional theory

L. Skuja[a], K. Smits[a], A. Trukhin[a], F. Gahbauer[b], R. Ferber[b], M. Auzinsh[b], L. Busaite[b], L. Razinkovas[c], M. Mackoit-Sinkevičienė[c], A. Alkauskas[c]

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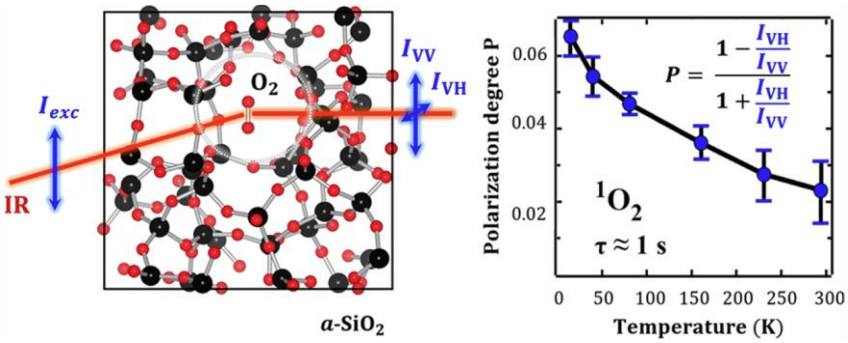
The lowest excited electronic state of the O_2 molecule, $a\ ^1\Delta_g$, the "singlet oxygen", is of utmost importance for photochemistry and photobiology. For O_2 trapped in silica glass, the lifetime of this state and the associated $a^1\Delta_g \longrightarrow X^3\Sigma_g^-$ photoluminescence (PL) is the longest known for O_2 in any condensed medium at room temperature. We studied the temperature dependence, decay kinetics and polarization anisotropy of this PL with 1064 nm excitation to the $a^1\Delta_g$ (v=1) state, as well as with excitation to higher energies. PL at this excitation shows non-zero polarization anisotropy at 295 K, which increases with cooling to 14 K. At variance, excitation to higher energies yields depolarized PL. Polarization data indicate weak electric dipole character of the emission of the spin- and parity-forbidden $a^1\Delta_g \longrightarrow X^3\Sigma_g^-$ transition, enabled by O_2 – SiO_2 cage interactions. Density functional theory calculations indicate that at low temperatures the rotation of O_2 is partially or fully frozen even in large silica voids. As the temperature increases, PL is increasingly depolarized by libration movement of O_2 molecules. Analysis of O_2 optical absorption in optical fibers allows one to obtain the absorption cross sections of $X \longrightarrow a$ and $X \longrightarrow b$ transitions of O_2 in SiO_2 glass and to evaluate both radiative and non-radiative rates of $a \longrightarrow X$ luminescence.



Interstitital O_2 molecule in interstitial site of SiO_2 glass network, excited by linearly polarized light, and temperature dependence of the polarization degree of singlet O_2 luminescence at 1272 nm, indicating hindered rotation of O_2 in SiO_2 glass.

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L. Skuja, K. Smits, A. Trukhin, F. Gahbauer, R. Ferber, M. Auzinsh, L. Busaite, L. Razinkovas, M. Mackoit-Sinkevičienė, A. Alkauskas, J. Phys. Chem. C 124 (2020) 7244-7253, doi:10.1021/acs.jpcc.9b11581.

II. Nanotechnology, thin films, nanocomposites and ceramics.

Structure properties of CdTe nanocrystals created in SiO_2/Si ion track templates

R. Balakhayeva[a], A. Akilbekov[a], Z. Baimukhanov[a], Sh. Giniyatova[a], M. Zdorovets[a,b,c], Y. Gorin[b], A.I. Popov[d,e], A. Dauletbekova[a]

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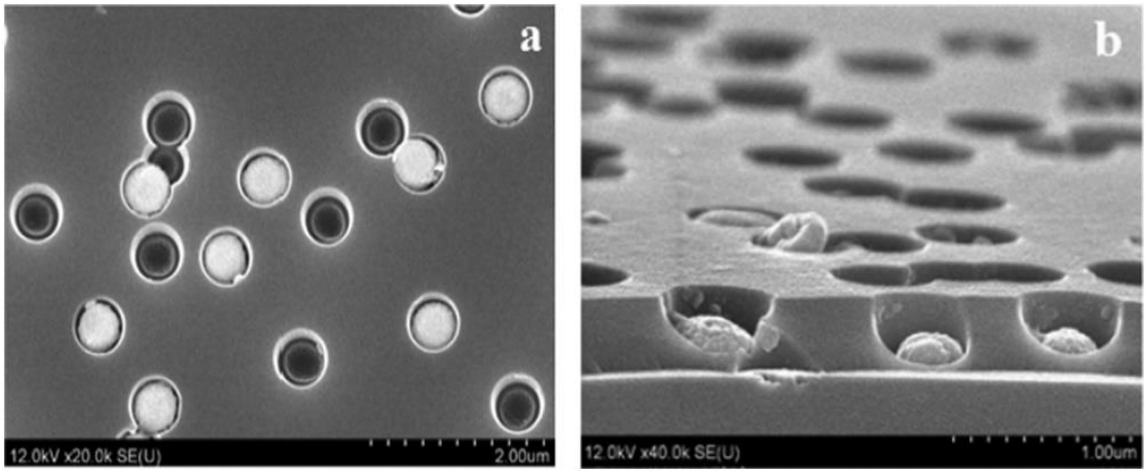
Currently, CdTe nanocrystals of the WS modification are considered one of the most promising for the production of highly efficient solar cells. In recent years, various types of CdTe nanoparticles were prepared by different chemical methods - through organometallic routes, by an exchange reaction between sodium telluride and cadmium iodide in methanol and by precipitation of Cd^{2+}-ions. The aim of this work is to carefully determine the synthesis conditions and their influence on the growth and morphology of CdTe nanocrystals, which are formed in a-SiO_2/Si ion track templates.The synthesis of CdTe nanocrystals was realized by electrochemical (ECD) and chemical (CD) deposition in SiO_2/Si-n structures irradiated with 200 MeV ^{132}Xe ions.



(a) and (b) SEM images of the frontal and cross section surfaces of the n-type template after CD CdTe at room temperature.

Both types of electrolyte (sulfate and chloride) used in ECD led to the formation of CdTe nanocrystals in single wurtzite phase. On the other hand, in the case of CD in a sulfate solution, CdTe nanocrystals with a zinc blende structure are formed that coexist with CdO nanocrystals in the hexagonal structure. Furthermore, an increase in the temperature of the CD solution led only to the formation of hexagonal phase of CdO nanocrystals. A model is proposed for the formation of a CdTe nanocrystal inside the ion track, taking into account the influence of a weak external electric field on the region of the inner surface of the ion tracks.

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R.Balakhayeva, A. Akilbekov, Z. Baimukhanov, S. Giniyatova, M. Zdorovets, Y. Gorin, A.I. Popov, A. Dauletbekova, Surface and Coatings Technology 401 (2020) 126269, doi:10.1016/j.surfcoat.2020.126269.

Fe and Zn co-substituted beta-tricalcium phosphate (β-TCP): Synthesis, structural, magnetic, mechanical and biological properties

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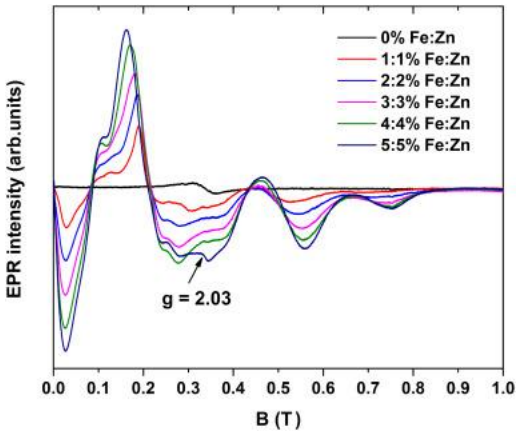
In the present study, Fe^{3+} and Zn^{2+} co-substituted β-tricalcium phosphate (β-TCP) has been synthesized by the wet co-precipitation method. Co-substitution level in the range from 1 to 5 mol% has been studied. Thermal decomposition of as-prepared precipitates was shown to be affected by the introduction of foreign ions, decreasing the decomposition temperature of a precursor. It was determined that partial substitution of Ca^{2+} by Fe^{3+} and Zn^{2+} ions leads to the change in lattice parameters, which gradually decreases as the doping level increases. Lattice distortion was also confirmed using Raman spectroscopy, which showed a gradual change of the peak shape in the Raman spectra. Rietveld refinement and electron paramagnetic resonance study confirmed that Fe^{3+} ions occupy only one Ca crystallographic site until Fe^{3+} and Zn^{2+} substitution level reaches 5 mol%. All co-substituted samples revealed paramagnetic behavior, the magnetization of powders was determined to be linearly dependent on the concentration of Fe^{3+} ions. Cytotoxicity of the synthesized species was estimated by *in vivo* assay using zebrafish (*Danio rerio*) and revealed the non-toxic nature of the samples. Preparation of ceramic bodies from the powders was performed, however, the results obtained on Vickers hardness of the ceramics did not show improvement in mechanical properties induced by co-substitution.



EPR spectra of TCP powders with different amounts of Fe and Zn.

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L. Sinusaite, A. Popov, A. Antuzevics, K. Mazeika, D. Baltrunas, J.-C. Yang, J. L. Horng, S. Shi, T. Sekino, K. Ishikawa, A. Kareiva, A. Zarkov, Mater. Sci. Eng. C 112 (2020) 110918, doi:10.1016/j.msec.2020.110918.

Growth and characterization of PbI_2-decorated ZnO nanowires for photodetection applications

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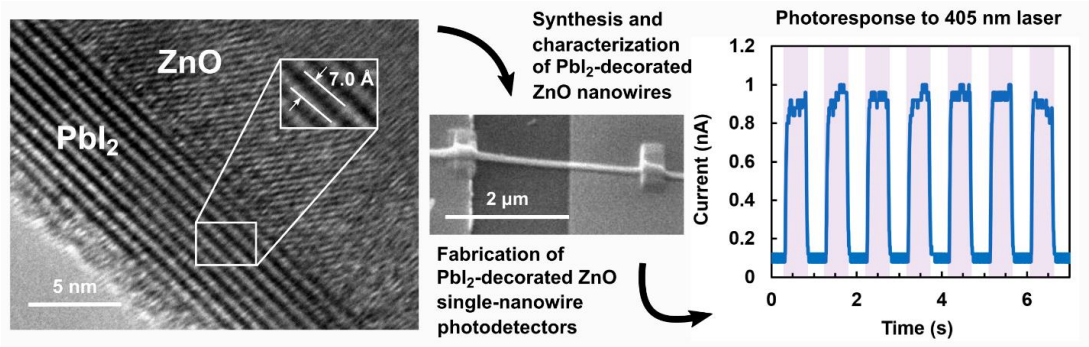
PbI_2, a layered van der Waals (vdW) material, similar to graphene and other transition metal dichalcogenides, such as MoS_2 and WSe_2, has been previously demonstrated as a potentially useful material for applications in optoelectronics due to its direct bandgap, as well as in X-ray detector devices. Controllable growth of uniform crystalline PbI_2 nanosheets is paramount for any emerging practical applications, thus we developed a novel two-step process including reactive magnetron deposition of a lead oxide film and subsequent iodination to PbI_2 on a ZnO NW substrate, and we compared as-grown hybrid nanostructures with ones prepared via thermal evaporation method.



In this study, we demonstrated for the first time growth of ZnO NWs decorated with highly crystalline few-layer PbI_2 and fabricated two-terminal single-nanowire photodetector devices to investigate the photoelectric properties of the novel hybrid nanostructures. In several studies, it has previously been demonstrated that passivating the ZnO NW surface or decorating the NW with specifically selected materials enhances the light and gas detecting properties. In this work, we showed that PbI_2-decorated ZnO NWs exhibit enhanced photoelectric properties in comparison to pure ZnO NWs - reduced dark current and decreased photoresponse time. The obtained results show the potential of combining layered vdW materials with semiconducting nanowires to create novel nanostructures with enhanced properties for applications in optoelectronics or X-ray detectors.

The produced nanostructures were characterized by scanning and transmission electron microscopy, X-ray diffraction analysis and photoluminescence measurements. Moreover, the experimental investigations were supported by total energy calculations of the electronic structure of both PbI_2 nanosheets and ZnO substrate. According to predictions made from our first principle calculations, such novel nanosized heterostructures might also be used for efficient photocatalytic and electrocatalytic hydrogen production from water due to their high surface-to-volume ratio.

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E. Butanovs, S. Piskunov, A. Zolotarjovs, B. Polyakov, J. Alloys Compd. 825 (2020) 154095, doi:10.1016/j.jallcom.2020.154095.

On the heuristic procedure to determine processing parameters in additive manufacturing based on materials extrusion

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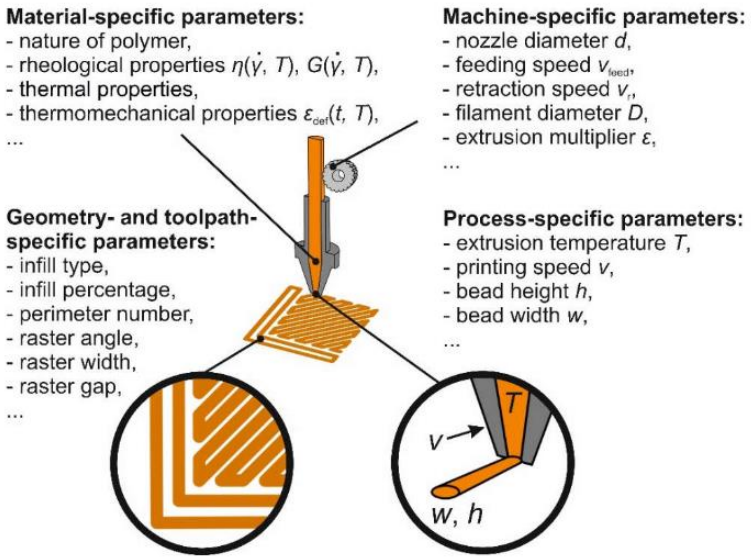
We present a heuristic procedure for determining key processing parameters (PPs) in materials-extrusion-based additive manufacturing processes. The concept relies on a design-of-experiment approach and consists of eleven "test objects" to determine the optimal combinations of key PPs values, starting with the PPs for printing the first layer and progressing to more complex geometric features, e.g., "bridges". In each of the test objects, several combinations of the known PPs'values are used, and only the values resulting in the best printed-part quality are selected for the following tests. The concept is intrinsically insensitive to different artifacts of the additive manufacturing machine (e.g., discrepancies between the nominal and actual nozzle diameters, and improper calibration of the feeding screws) and the optimal values of key PPs for manufacturing defect-free parts under the actual processing conditions can be determined. We validated the proposed procedure for two common commercial polymer feedstock materials, and we show that, by using the proposed procedure, it is possible to reduce the optimization time down to several hours, as well as to reduce the amount of consumed feedstock material. Tensile tests revealed a strong effect of the amorphous and semi-crystalline nature of the polymer on the results of optimization. To the best of our knowledge, this is the first attempt to describe a systematic approach for optimizing PPs for materials extrusion-based additive manufacturing processes without relying on statistical data analysis or virtual simulations. The concept was implemented as a web-tool 3DOptimizer®.



A diagram to illustrate different parameters in a material-extrusion-based additive manufacturing process.

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G. Bakradze, E. Arājs, S. Gaidukovs, V. K. Thakur, Polymers 12 (2020) 3009, doi:10.3390/polym12123009.

Impact of gadolinium on the structure and magnetic properties of nanocrystalline powders of iron oxides produced by the extraction-pyrolytic method

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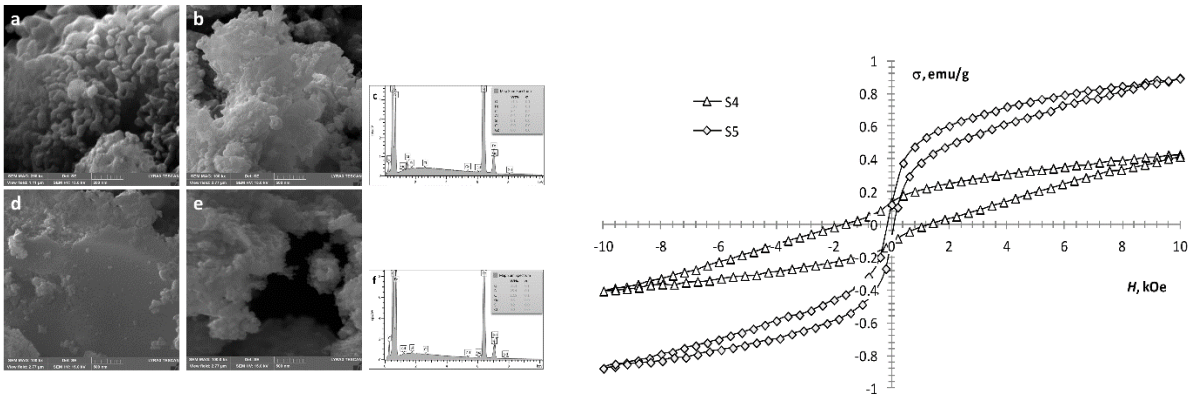
Interest in magnetic nanoparticles is primarily due to their broad practical applications. In this work, for the production of nanocrystalline powders of pure and gadolinium doped iron oxides, the extraction-pyrolytic method (EPM) was used. As a precursor, either iron-containing extract (iron (III) caproate in caproic acid) or its mixture with gadolinium-containing extract (gadolinium (III) valerate in valeric acid) was used. The mixed precursor contained 0.5 mol%, 2.5 mol%, 12.5 mol%, 50 mol%, and 75 mol% gadolinium in relation to the iron content. The formation of iron oxide phases, depending on the preparation conditions, was investigated. According to the results obtained, it was demonstrated that the presence of more than 2.5 mol% gadolinium additive in the mixed precursor inhibits the magnetite-to-hematite transformation process during thermal treatment. Produced samples were characterized by XRD and SEM methods, and the magnetic properties were studied moments analysis in order to identify the ground state configuration.



Left panel: SEM images and EDX spectrum of powders produced at 550 °C: (a–c)—S4 (undoped Fe_2O_3); (d–f)—S5 (0.5 mol% Gd-doped Fe_2O_3).
Right panel: Magnetization loops of samples S4 (undoped Fe_2O_3) and S5 (0.5 mol% Gd-doped Fe_2O_3).

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V. Serga, R. Burve, M. Maiorov, A. Krumina, R. Skaudžius, A. Zarkov, A. Kareiva, A.I. Popov, Materials 13 (2020) 4147, doi:10.3390/ma13184147.

Understanding the conversion process of magnetron-deposited thin films of amorphous ReO_x to crystalline ReO_3 upon thermal annealing

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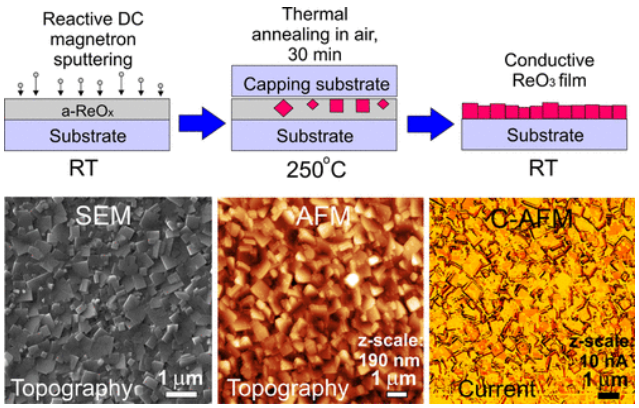
A comprehensive investigation of rhenium oxide thin film growth was performed to elucidate the mechanisms of ReO_3 formation upon thermal annealing from amorphous ReO_x produced by reactive DC magnetron sputtering. We found that the as-prepared films are X-ray amorphous but readily crystallize upon being annealed in the range of temperatures from 200 to 350°C. Nanocrystalline single-phase ReO_3 films were produced when heated to about 250°C. The nanocrystalline morphology of the annealed films was evidenced by XRD spectroscopy, scanning and transmission electron microscopy, and atomic force microscopy. The metallic nature of the films was confirmed by macro- and nanoscale conductivity measurements. The ReO_3 films demonstrated optical properties typical for thin metallic layers. They appeared bright red in reflected light and blue-green in transmitted light, being transparent in the spectral range of 475−525 nm.

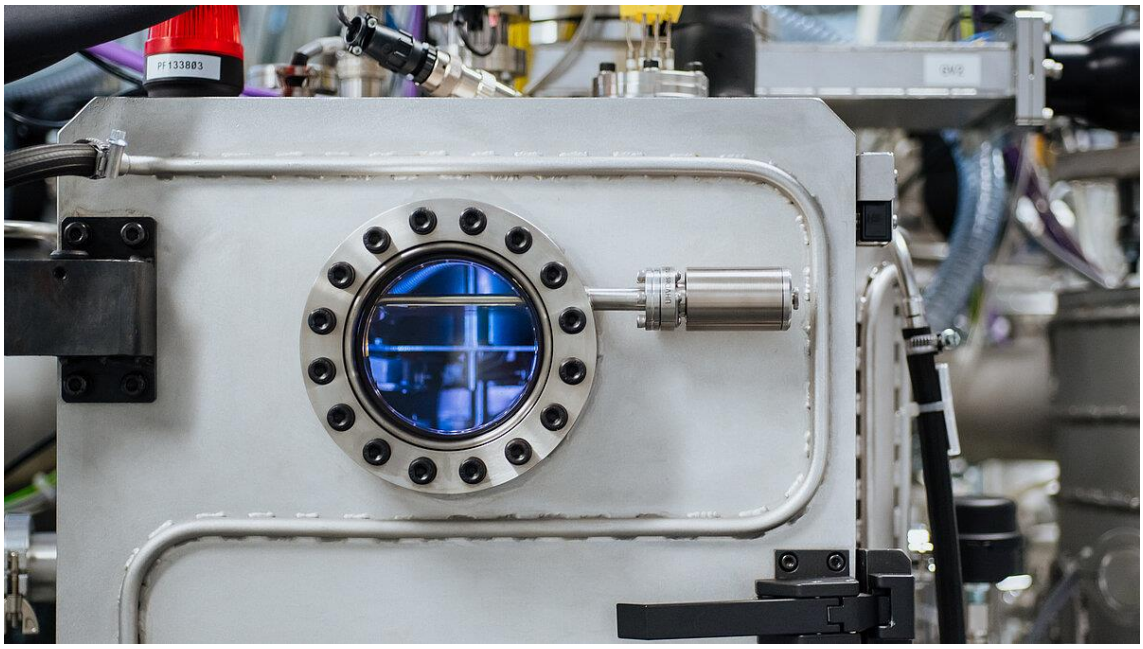


The conversion process of amorphous ReO_x thin film to crystalline ReO_3 upon thermal annealing.

The local atomic structure of the films was studied by X-ray absorption spectroscopy (XANES/EXAFS). The analysis of the Re L_3-edge EXAFS spectra using the reverse Monte Carlo method suggested that the local atomic structure around rhenium atoms in the as-prepared films was strongly disordered and resembled that in o-ReO_2, whereas the local structure of the thin film annealed in the air at 250°C was close to the one in crystalline c-ReO_3 but slightly more disordered, reflecting the nanocrystalline morphology of the films. The oxidation state of the rhenium ions was close to 4+ in the as-prepared film and 6+ in the annealed one, which was confirmed by XANES and X-ray photoemission spectroscopies. The obtained results allowed us to understand the mechanism of rhenium oxide conversion from the initially amorphous ReO_x phase to cubic crystalline ReO_3 when annealed.

Published in:
B. Polyakov, E. Butanovs, A. Ogurcovs, S. Vlassov, M. Zubkins, I. Jonane, A. Cintins, A. Kalinko, A. Kuzmin, J. Purans, Cryst. Growth Des. 20 (2020) 6147-6156, doi:10.1021/acs.cgd.0c00848.

III. Functional materials for photonics and electronics.



Anisotropic photoluminescence of nonpolar ZnO epilayers and $ZnO/Zn_{1-x}Mg_xO$ multiple quantum wells grown on $LiGaO_2$ substrate

T. Yan[a,b], L. Trinkler[c], V. Korsaks[c], C.-Y. J. Lu[a], B.Berzina[c], L. Chang[a], M. M. C. Chou[a], K. H. Ploog[a]

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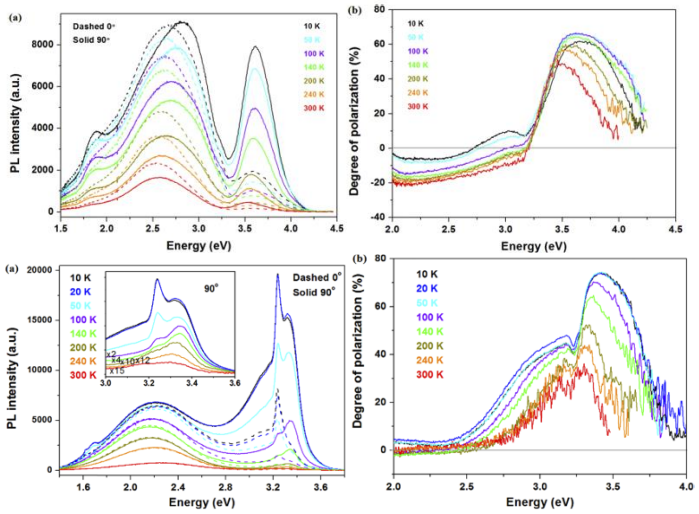
Nonpolar ZnO heterostructures exhibit two major advantages. First, the heterostructures are free from the spontaneous polarization fields in the growth direction. The quantum-confined Stark effect and the associated red shift of the near band-edge emission can be avoided. Second, the heterostructures exhibit intrinsically an in-plane optical anisotropy according to the polarization selection rules. Due to these two characteristics, light-emitting devices fabricated from nonpolar ZnO heterostructures can find unique applications such as the backlight for liquid crystal displays. Besides, the optical anisotropy can be utilized in polarized light emission, polarization-sensitive photodetector, the converter in optical communication, nonlinear optical component, and gas sensing.

Polarised photoluminescence was studied under excitation with 263 nm laser in 10-300 K range for m- and a-plane ZnO epilayers grown on $LiGaO_2$ substrates.

The m-plane ZnO epilayer exhibits a weak anisotropy with the degree of polarization of 30% for basal stacking faults (BSFs) and 10% for the near band edge (NBE)emission at 10 K, which is nearly absent at room temperature. The degree of polarization of m-plane quantum wells (QWs) changes from 76% at 10K to 40% at 300 K. The strong anisotropy might be attributed to the enhanced confinement effect of a one-dimension confinement structure caused by the intersection of QW and BSF. In addition to the temperature, the degree of polarization was also influenced by the polarization of the exciting laser beam. As for the a-plane ZnO epilayer, the degree of polarization of 74% for the NBE emission is higher than that of 42% for BSFs at 10 K, which decreases to 33% and 25% at 300 K, respectively. It is assumed that the luminescence polarization should be affected not only by the in-plane strains but also the microstructural defects, which do modify the electronic band structure.



(a) 0° and 90° Polarized PL spectra, (b) the corresponding degree of polarization, of the m-plane ZnO QWs (above) and the a-plane ZnO epilayer (below) at 10-300 K.

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T. Yan, L. Trinkler, V. Korsaks, C.-Y.J. Lu, B.Berzina, L. Chang, M.M.C. Chou, K.H. Ploog, Optics Express, 28 (2020) 5629-5638, doi:10.1364/OE.385828.

Luminescence and vacuum ultraviolet excitation spectroscopy of samarium doped SrB_4O_7

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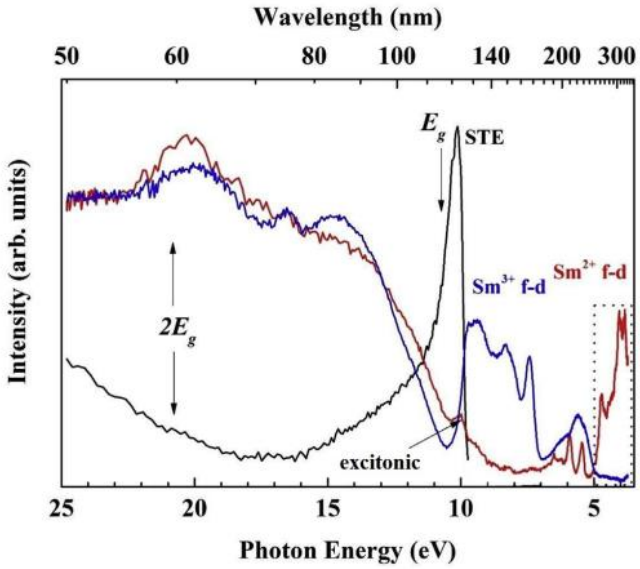
Sm^{2+} and Sm^{3+} co-doped SrB_4O_7 could be utilized in several high-level optical devices and fundamental knowledge about the optical behavior of these materials benefits the development of luminescent applications.

In current work we report a systematical investigation of Sm^{2+} and Sm^{3+} co-doped SrB_4O_7. Synchrotron radiation-induced luminescence and vacuum ultraviolet (VUV) excitation spectra were recorded to study charge migrations during the de-excitation and excitation processes within the doped systems. The experimental results have been compared to the partial density of states (PDOS) calculations conducted for pure, as well as Sm^{2+}- and Sm^{3+}-doped SrB_4O. Results of the luminescence emission measurements show that depending on the excitation energy, the observed emission is related to either Sm^{2+} or Sm^{3+}. Additionally, intrinsic emission was detected in SrB_4O_7 and attributed to the selftrapped exciton (STE). To our best knowledge, this type of behavior in SrB_4O_7 has not been reported before. The analysis about the STE emission was indirectly confirmed through excitation spectra and an intensive STE excitation band was detected at around 10 eV, which is close to the calculated band gap value of SrB_4O_7. Furthermore, charge multiplication processes were detected at energies higher than 20 eV (about $2E_g$) by further growth of the excitation curve. Additionally, the experimental excitation spectra showed inter-configurational Sm^{2+} and Sm^{3+} f-d-transitions and our calculations support the experimental observations. In summary, this study clarified excitation and emission behavior of samarium doped SrB_4O_7 with coherent results between our experimental results and first-principles calculations.



The excitation spectra of Sm^{2+} ($^5D_0$-$^7F_0$ at 684 nm, red), Sm^{3+} ($^4G_{5/2}$-$^6H_{7/2}$ at 590 nm, blue) and intrinsic (300 nm, black) emissions in SrB_4O_7:Sm (0.5%) at 10 K.

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A. Tuomela, Meng Zhang, M. Huttula, S. Sakirzanovas, A. Kareiva, A.I. Popov, A.P. Kozlova, S. Assa Aravindh, W. Cao, V. Pankratov, J. Alloys Compd 826 (2020) 154205, doi: 10.1016/j.jallcom.2020.154205.

Time-resolved luminescence and excitation spectroscopy of co-doped $Gd_3Ga_3Al_2O_{12}$ scintillating crystals

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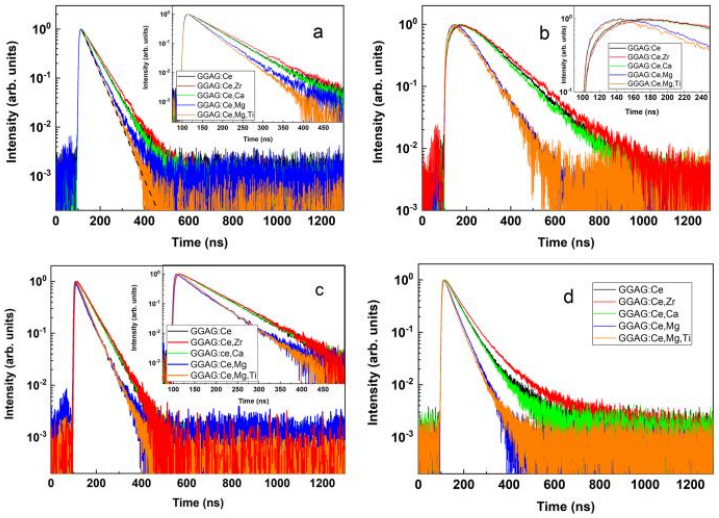
Among other scintillator materials cerium doped gallium gadolinium aluminum garnet ($Gd_3Ga_3Al_2O_{12}$:Ce or GGAG:Ce) nowadays is one of the most relevant scintillator materials because it comprises the combination of such properties, as a very high light output of scintillations, high density, and relatively fast decay time,. Furthermore, this material is very suitable for neutron detection and discrimination, thanks to the high Gd cross-section for neutron interaction.

The luminescence properties of cerium doped as well as co-doped GGAG single crystals have been investigated by means of time-resolved luminescence spectroscopy under tunable laser excitations. It is suggested that the Mg^{2+} co-doping strongly suppresses intrinsic defects in GGAG:Ce single crystals removing competing relaxation channels of hot charge carriers. The combination of time-resolved luminescence spectroscopy and excitation spectroscopy techniques allows to conclude that the excitation band of Ce^{3+} emission peaking at about 235 nm (5.3 eV) is due to $4f–5d_3$ transitions in Ce^{3+} ion in GGAG crystals. It was observed that Ce^{3+} luminescence decay is faster in the Mg^{2+} co-doped crystals under any photo excitations below the energy of band-to-band transitions in the GGAG. It means that improved scintillating properties of Mg^{2+} co-doped GGAG:Ce crystals known in literature are driven not only by the formation of luminescence center from Ce^{4+} ion but also by the perturbation of Ce^{3+} ion by Mg^{2+} co-dopants.



Luminescence decay kinetics of the Ce3+ emission (530 nm) in the co-doped GGAG:Ce single crystals under 450 nm (a), 275 nm (b), 235 nm (c) and 210 nm (d) excitations at room temperature. Black dashed line in (a) demonstrates an example of single exponential fit if the parameter of the decay time constantis 40 ns.

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V. Pankratova, A.P.Kozlova, O.A. Buzanov, K. Chernenko, R. Shendrik, A. Šarakovskis, V. Pankratov, Scientific Reports 10 (2020)20388, DOI: 10.1038/s41598-020-77451-x.

Luminescence and vacuum ultraviolet excitation spectroscopy of cerium doped $Gd_3Ga_3Al_2O_{12}$ single crystalline scintillators under synchrotron radiation excitations

A.P.Kozlova[a], V.M. Kasimova[a], O.A. Buzanov[b], K. Chernenko[c], K. Klementiev[c], V. Pankratov[d]

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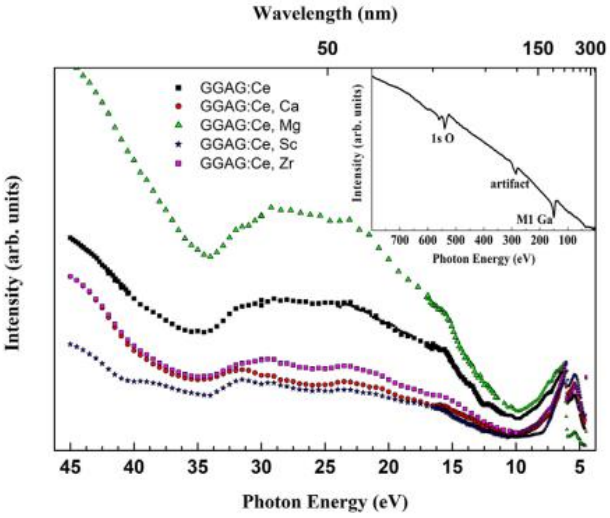
Cerium doped Gallium Gadolinium Aluminum Garnet ($Gd_3Ga_3Al_2O_{12}$:Ce or GGAG:Ce) nowadays is one of the most popular scintillation material. GGAG:Ce demonstrates excellent light output of scintillations (58,000 photons/MeV) and, therefore, it is considered to be as one of the most prospective scintillators in high energy physics as well as in medical applications.

The luminescence properties of cerium doped as well as co-doped GGAG single crystals have been investigated by means of the vacuum ultraviolet (VUV) excitation spectroscopy utilizing radiation from the undulator beamline (FinestBeaMS) of 3rd generation synchrotron facility MAX IV. These results were supported by XANES experiments identifying Ce^{3+} and Ce^{4+} centers in the co-doped GGAG crystals. The pioneering luminescence results have been obtained for the GGAG:Ce single crystals in VUV and soft X-ray excitation range. It was shown that GGAG:Ce single crystals having different co-dopant ions reveal distinguished efficiency of multiplication electronic excitations in VUV spectral range. Two models were proposed to explain the differences in the excitation efficiency for the crystals studied. The first one proposes that co-dopants can influence a thermalization length of geminate electrons and holes. Another one suggests that intrinsic defects in GGAG lattice are responsible for the capture of hot charge carriers leading to the degradation of the excitation efficiency in VUV spectral range. It is also suggested that the luminescence properties can be improved by the co-doping of Mg^{2+} ions suppressing intrinsic defects in GGAG:Ce single crystals, which are responsible for the excitation band at 5.3 eV as well as for the capture of hot charge carriers influencing the excitation region in VUV range and restricting scintillating performance of GGAG:Ce.



The excitation spectra of Ce^{3+} emission (530 nm) in VUV spectral range for the co-doped GGAG:Ce single crystals at 10 K. The excitation spectrum extended to 800 eV for the GGAG:Ce non-co-doped single crystal is shown inset.

Published in:
A.P.Kozlova, V.M. Kasimova, O.A. Buzanov, K. Chernenko, K. Klementiev, V. Pankratov, Results in Physics 16 (2020) 103002, doi: 10.1016/j.rinp.2020.103002.

The boron effect on low-temperature luminescence of $SrAl_2O_4$:Eu,Dy

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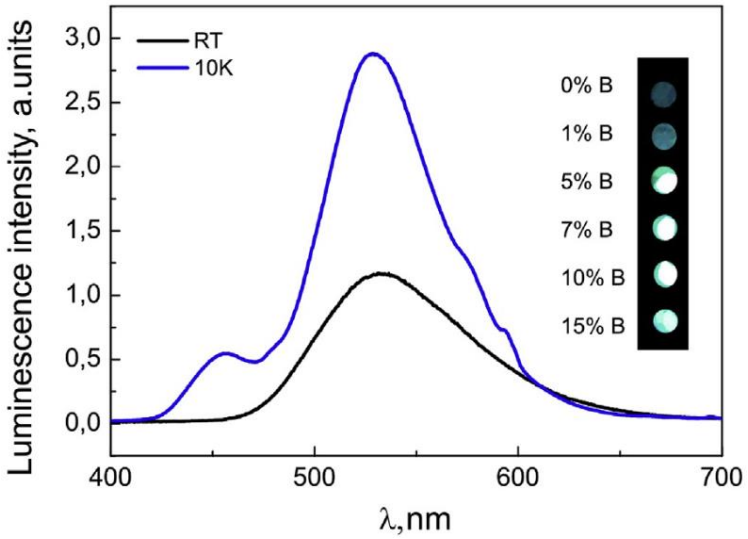
Temperature dependence of the afterglow of persistent luminescence material $SrAl_2O_4$:Eu,Dy is a major problem for outdoor low-temperature applications. Therefore this publication deals with tailoring the material for better outdoor use by exploring the second mechanism, which is involved in the afterglow – charge tunnelling from the trapping center to the luminescence center. Structure, morphology, emission and thermally stimulated luminescence properties have been measured for $SrAl_2O_4$:Eu,Dy samples with different added boron percentages. The results indicate a change in morphology of the samples with increasing boron concentration, as well as a change in afterglow times. The low-temperature luminescence intensity and afterglow time dependence of boron addition turns out to be different from the room temperature luminescence intensity and afterglow time dependence from boron concentration. Boron addition in the necessary amount plays a key role in creating trapping centers in the material that are located spatially close to the luminescence center thus making the material afterglow possible even in low temperatures.

The boron incorporation in the $SrAl_2O_4$:Eu,Dy material contributes to the creation of the trapping center, leading to prolonged afterglow times. However, these trapping centers are in spatially different positions – some are located in such positions, that the tunnelling from the trapping center is possible, but some – located too far for the probability of tunnelling to be substantial. Adding boron above 7 at% in our experiments leads to the creation of spatially further located trapping centers, therefore the samples with large boron concentrations do not exhibit afterglow at lower temperatures. This leads to a conclusion that the luminophores can be modified intentionally to create long afterglow materials more suited for outdoor use.



The emission spectrum of $SrAl_2O_4$: Eu,Dy with 5 at% B addition right after the termination of excitation at room temperature and 10 K temperature.

Published in:
V. Vitola, I. Bite, D. Millers, A. Zolotarjovs, K. Laganovska, K. Smits, A. Spustaka, Ceramics International 46 (2020) 26377-26381, doi:10.1016/j.ceramint.2020.01.208.

Defect-related photoluminescence and photoluminescence excitation as a method to study the excitonic bandgap of AlN epitaxial layers: Experimental and ab initio analysis

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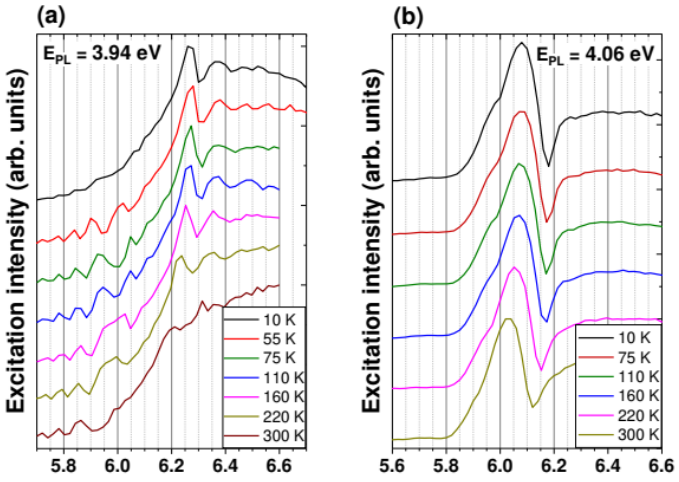
We report defect-related photoluminescence (PL), and its vacuum ultraviolet (VUV) photoluminescence excitation (PLE) spectra of aluminum nitride layers with various layer thicknesses and dislocation densities grown on two different substrates: sapphire and silicon. The defect-related transitions have been distinguished and examined in the emission and the excitation spectra investigated under synchrotron radiation. The broad PL bands of two defect levels in the AlN were detected at around 3 eV and 4 eV. In the PLE spectra of these bands, sharp excitonic peak originating the most probably from the A-exciton of AlN was clearly visible. Taking into account the exciton binding energy, the measurements allow determination of the bandgaps of the investigated AlN samples and their temperature dependencies. Next, they are compared with the literature data obtained by other experimental techniques for bulk AlN crystals and layers grown on different substrates. The obtained results revealed that the AlN bandgap depends on the substrate. The theoretical analysis using density functional theory (DFT) calculations showed that the effect is induced by the tetragonal strain related to the lattice mismatch between the substrate and the AlN layer, which has a strong influence on the spectral positions of the intrinsic excitons, and consequently on the bandgap of AlN layers.



Temperature dependence of the PLE spectra of the AlN layers on (a) sapphire and (b) silicon substrates, monitored at defect-related emission energy of around 4 eV.

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A. Kaminska, K.l Koronski, P.l Strak, A. Wierzbicka, M. Sobanska, K. Klosek, D.V. Nechaev, V. Pankratov, K. Chernenko, S, Krukowski, Z.R. Zytkiewicz, Appl. Phys. Lett. 117 (2020) 232101, doi: 10.1063/5.0027743.

Low temperature X-ray absorption spectroscopy study of $CuMoO_4$ and $CuMo_{0.90}W_{0.10}O_4$ using reverse Monte-Carlo method

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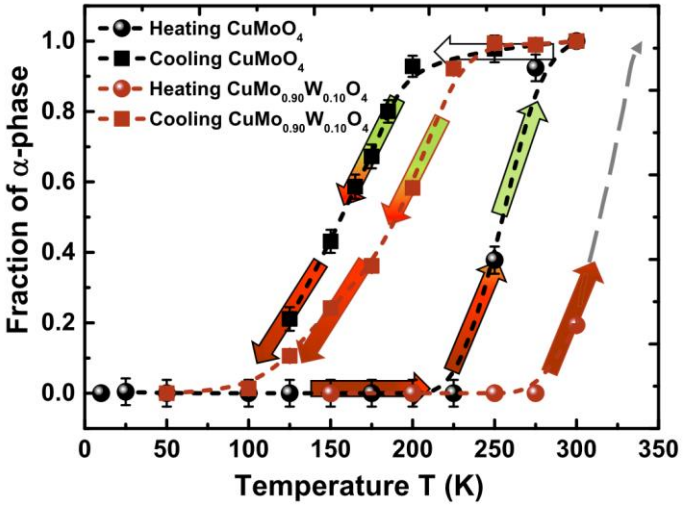
Copper molybdate ($CuMoO_4$) exhibits thermochromism and piezochromism originated from the first-order structural phase transition accompanied by a drastic colour change between green and brownish-red. Furthermore, the phase transition temperature can be increased by inducing chemical pressure upon substitution of molybdenum ions with tungsten ones. Depending on the tungsten concentration in $CuMo_{1-x}W_xO_4$ solid solutions, phases isostructural to high-pressure $CuMoO_4$ can be obtained. The most attractive for technological applications compound in the solid solution series is $CuMo_{0.90}W_{0.10}O_4$, because of its ability to switch between the two allotropic forms (α and γ) in the temperature range from 0 to 100°C.

To better understand the structure-property relationships in $CuMo_{1-x}W_xO_4$ solid solutions, X-ray absorption spectroscopy was used to probe a variation of the local atomic structure in $CuMoO_4$ and $CuMo_{0.90}W_{0.10}O_4$ in the temperature range of 10–300 K.



Temperature dependence of the fraction of α phase in $CuMoO_4$ and $CuMo_{0.90}W_{0.10}O_4$ samples upon heating and cooling. The gray dashed line with an arrow is an extrapolation above the room temperature for $CuMo_{0.90}W_{0.10}O_4$.

Extended X-ray absorption fine structure (EXAFS) data analysis of $CuMoO_4$ and $CuMo_{0.90}W_{0.10}O_4$ is a challenging task due to the low symmetry of the α and γ phases, leading to a distortion of the local environment. In such a case, the conventional EXAFS analysis is less effective because of the large number of fitting parameters required. Advanced data analysis of EXAFS spectra at several absorption edges (K-Cu, K-Mo and L_3-W) simultaneously interpreted by reverse Monte Carlo method allowed us to monitor the α-to-γ and γ-to-α thermochromic phase transitions, occurring gradually with the two-phase co-existence range. We observed that the addition of 10 mol% of tungsten to $CuMoO_4$ induces local distortions and stabilizes the γ-phase, leading to an increase of the phase transition temperature by about 50–100 K.

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I. Jonane, A. Cintins, A. Kalinko, R. Chernikov, A. Kuzmin, Rad. Phys. Chem. 175 (2020) 108411, doi:10.1016/j.radphyschem.2019.108411.

Phase retrieval of a Kolmogorov phase screen from very sparse data using four binary masks

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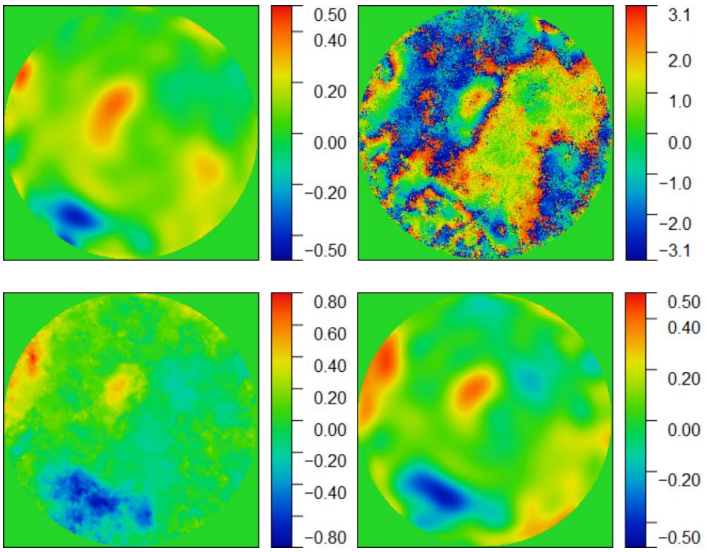
Astronomical adaptive optics deals with improving the optical quality of astronomical images based on the correction of a wavefront. Various methods have been proposed to measure the shape of a wavefront. The most popular method is the Shack-Hartmann aberrometry. However, in recent years various phase retrieval methods have become increasingly popular for measuring the shape of a wavefront. In the current study, we investigate the phase retrieval of a Kolmogorov phase screen or the phase map of a turbulent atmosphere encountered in astronomical adaptive optics.

The phase retrieval algorithm called PhaseLift and used in the study is based on retrieving the phase of the object under study from a very limited number of coded diffraction patterns. The object is modulated with four binary amplitude modulating masks which are rotated versions of each other. The coded diffraction patterns are acquired with a camera of low bit depth (10-bits). PhaseLift is an optimization algorithm based on low-rank Riemannian optimization methods.



The Kolmogorov phase screen retrieved with the surface profiler and PhaseLift. See the text for details. After subtracting the phase screen measured with the profiler from that retrieved with PhaseLift, the root-mean-square error decreased and the Strehl ratio increased.

The Kolmogorov phase screen retrieved with PhaseLiuft was compared to that measured with a non-contact surface profiler. The results are shown in Figure. The top-left panel shows the phase screen measured with the profiler (in micrometers), the top-right shows the phase screen retrieved with PhaseLift and wrapped from -π to +π, the bottom-left panel shows the unwrapped phase screen (in micrometers) and the bottom-right panel shows a smoothed phase screen (in micrometers). The data has been obtained at the He-Ne laser wavelength (l=0.6328 μm). After subtracting the phase screen measured with the profiler from that retrieved with PhaseLift, the root-mean-square error decreased from 0.14 to 0.10 μm, and the Strehl ratio increased from 0.14 to 0.37.

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V. Karitans, K. Laganovksa, K. Kundzins, Appl. Opt. 59 (2020), 8362-8369, doi:10.1364/AO.399018.

Visual acuity, colour discrimination in patient with cataract

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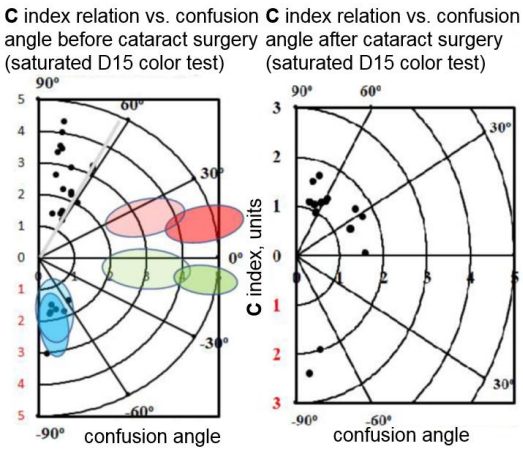
Solid state optical systems use various light detectors with accurate continuous output. Biological systems determine output using psychophysical principles. However psychophysical methods allow to judge on bio-media optical quality. This quality changes with aging (as in the case of ocular lens cataracts), and merits such as changes in the sensitivity of photoreceptors in the eye can cause a variety of side effects in the elderly. Various methods are used to transform patient judgments into objective optical indicators. We used saturated Farnsworth D15 Color vision arrangement test to check colour sensitivity changes in retina photoreceptor confusion line directions. It is easily perceptible (essential to elder patients), and it is possible to check colour sensitivity changes in tritan, protan and deutan confusion line directions. The results were analyzed in three ways: by summing the colour differences between adjacent test caps according to Bowman; averaging colour difference vectors according to Vingry and King – Smith; using linear regression line made from error cap arrangements (LSR method).

Using Farnsworth D15 arrangement analysis methods: inertia moment method, Bowman method and Least square method, we conclude that test helps to observe changes of color discrimination, thus the optical density of the cataract. All three analysis showed that cataract caused lens opacity's decrease significantly in visible light chromatic resolution. Based on intraocular lens examination in biomicroscopy prior to cataract operation and colour arrangement test results before and after surgery, it could be suggested chromatic sensitivity decrease along tritan axis was observed due to significantly increased absorption in intraocular lens. Before the cataract surgery, the D15 test stimulus arrangement sequence showed similarities with the tritan colour deficiency. Patient arrangement of colored dice sequence and Bowman developed scale is easy and quick for specialist who is performing vision function tests. D15 test can be a test which can give as information about drugs and other eye pathology's influence on preretinal absorption. Higher grade cataract can cause color vision sensitivity changes.



Patients D15 colour arrangement sequence corresponding confusion index (C index) and confusion angle (degrees) before and after cataract surgery. Area with C < 2 corresponds to photoreceptor good color discrimination. In cases of protan, deutan and tritan photoreceptor deficiency analysis points lie along corresponding confusion line directions and C values are inside diagram colored areas – for light or severe photoreceptor deficiency.

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Z. Langina-Jansone, R. Truksa, M. Ozolinsh, J. Optical Society of America A 37 (2020) A212-A216, doi: 10.1364/JOSAA.382397.

Pyroelectric activity of $LiGaO_2$, Li_2GeO_3, $Li_2B_4O_7$ and $LiNbO_3$ crystals: pyroelectric luminescence and excitation of cathodoluminescence in scintillator $ScPO_4$

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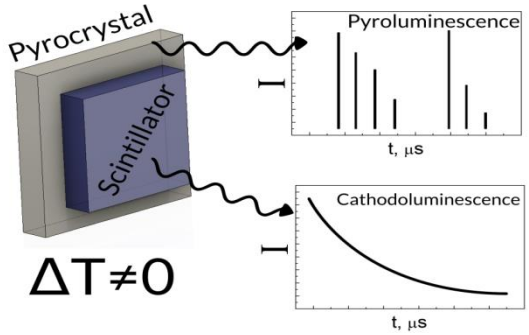
Pyroelectric luminescence (PEL) is observed as spontaneous luminescence without any external excitation in some noncentrosymmetric crystals, when a rapid change of temperature causes changes in electric polarization due to thermal distortion of the crystal lattice and failure of free charge carriers, gathering on the crystal surface, to compensate the pyroelectric field and bursting into dielectric discharge followed by luminescence process both inside and outside the pyroelectric crystal. It was even assumed that the high voltage crystal field (up to 100 kV) in the pyroelectric crystal can cause X-ray generation. First of all we have studied the properties of the known pyroelectric crystals, β-$LiGaO_2$, Li_2GeO_3, $Li_2B_4O_7$ and $LiNbO_3$, recording electron emission and kinetic and spectral features of PEL occurring during fast cooling and heating runs, thus obtaining typical PEL characteristics. To understand how the pyroelectric activity is affecting the environmental medium, as luminescent agents we have used scintillators, which are not pyroelectric crystals and give no spontaneous luminescence signal when cooled/heated by themselves.



Crystals $LiGaO_2$, Li_2GeO_3, $Li_2B_4O_7$ and $LiNbO_3$ exhibit pyroelectric luminescence and electron emission with a change of temperature. Pyroelectric luminescence spikes are fast in the range of nanosecond. Pyroelectric activity of the crystals excites luminescence of a scintillator crystal $ScPO_4$.

Analysing the experimental results on luminescence, induced by pyroelectric effect in "pyrocrystal + $ScPO_4$" pairs the following compilation can be done. Compared to PEL from a pyrocrystal alone, luminescence signal from a pair with an attached $ScPO_4$ crystal 1) is much more intense (up to two orders of magnitude); 2) luminescence spectra reveal features of the doped $ScPO_4$ luminescence in the visible range and demonstrate STE band of this crystal at 210 nm; 3) kinetic measurements taken in the UV range show luminescence decay pulse having a fast (several ns) and a slow (several μs) components, typical to STE luminescence of $ScPO_4$ crystal in PL and (CL), which is dissimilar to PEL kinetics of pyrocrystals, characterized with individual spikes in the nanosecond range. Besides $ScPO_4$, other scintillator materials like pure and doped SiO_2 crystals and glasses were tried in pair with pyrocrystals. The results were similar: pyroelectric activity of pyroelectrics caused luminescence of scintillators with kinetic parameters typical to scintillators' PL and CL. Two aspects of practical use of a "Pyrocrystal + Scintillator" pair: 1) a scintillator enhances the PEL signal from a pyrocrystal thus facilitating its detection; 2) a pyroelectric crystal serves as a pulsed source of electrons useful for luminescence excitation in scintillator materials in specific conditions.

Published in:
I. A. Trukhin, L. Trinkler, A. Zolotarjovs, Opt. Mat. 109 (2020) 110391, doi:10.1016/j.optmat.2020.110391.

Nitrogen vacancy type defect luminescence of AlN nanopowder

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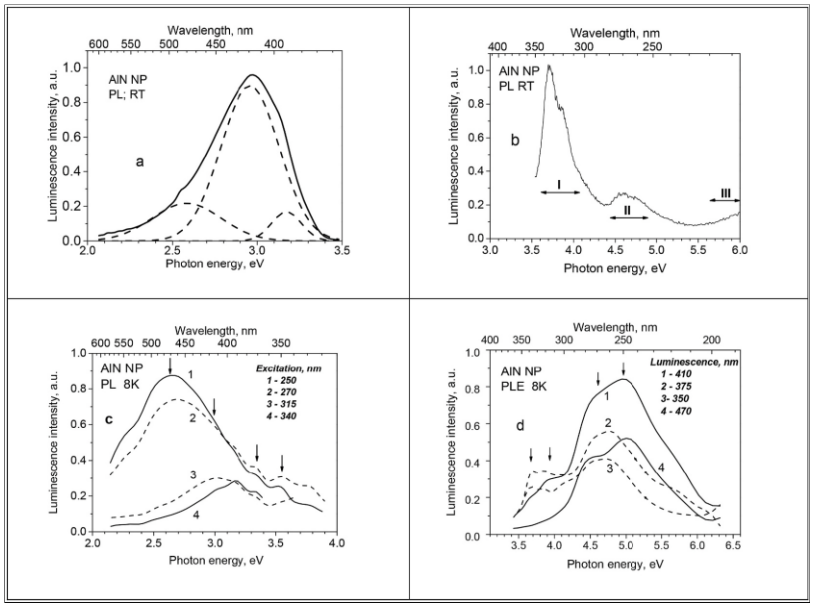
Aluminum nitride (AlN) is a prospective direct wide band gap semi-conductor with an energy gap around 6.0 eV and wurtzite structure, which is presenting several excellent properties, such as high thermal conductivity (~300 $Wm^{-1}K^{-1}$) and consistent physical and chemical stability. Besides, AlN possesses promising optical properties, which stimulated the elaboration of far-ultraviolet (UV) light emitter based on excitonic processes, as well as demonstrating prospective qualities for UV light dosimeter based on the luminescence of oxygen-related native defects.

Experimental investigation of native luminescent defects of AlN NP was performed by studying luminescence and its excitation spectra within a wide spectral region including UV and visible light and temperature interval from 8 K to RT. Excitation was provided either by a deuterium lamp or by a solid-state laser 263 nm.



AlN NP Photoluminescence spectra (a, and c) and luminescence excitation spectra (b and d) at RT and 8 K, respectively. a – PL spectrum at 315 nm or 260 nm excitation; b – PLE spectrum of BL at RT, where three spectral intervals are marked (I, II and III). c - PL spectra at 8 K under different excitations. d – PLE spectra at 8 K for different luminescence intervals.

A wide and complex luminescence band was observed in the blue spectral region, consisting of the sub-bands at 390 nm and 415 nm with similar spectral characteristics. It was found that the blue luminescence (BL) can be caused by several mechanisms including intra-center and recombination luminescence mechanism as well as energy transfer from excitons of the host material, which are dependent on the spectral region of the exciting light. Analysis of the results of spectral measurements and its comparison with those from the literature data allow the assignment of the native defects causing the BL in AlN NP to F-center type defects based on VN. These defects are located both in the bulk of the material and on its surface. The BL caused by the surface defects is sensitive to environmental oxygen gas which is reducing the intensity of the BL.

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B. Berzina, L. Trinkler, V. Korsaks, R. Ruska, Optical Materials, 108 (2020) 110069, doi:10.1016/j.optmat.2019.109529.

Recombination luminescence of X-ray induced paramagnetic defects in BaY_2F_8

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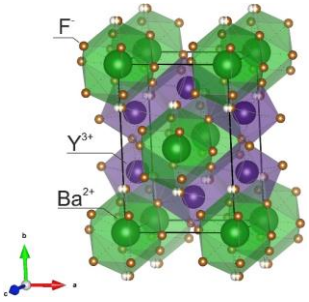
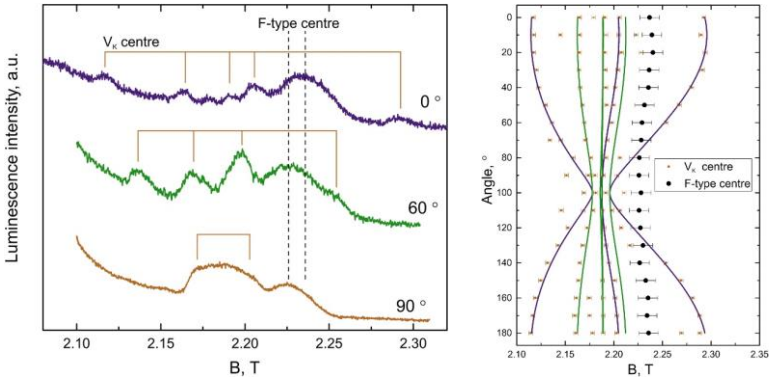
Monoclinic barium yttrium fluoride (BaY_2F_8) has been widely investigated as an optical material due to its high transparency, low phonon energy and low symmetry nature of the lattice. When doped with rare earth (RE) ions, BaY_2F_8 is best-known for its stimulated emission in lasers, however other applications such as scintillators, optical refrigerators and up-conversion coatings for solar cells have shown promise as well.

Efficiency of luminescence processes in materials is affected by the local structure of RE ions as well as the presence of intrinsic defects in the lattice. Although the interest in BaY_2F_8 is high, there is a relatively low number of studies focusing on the characterization of defect local structure, especially with methods, which involve magnetic resonance techniques. The lack of magnetic resonance investigations of BaY_2F_8 can be explained by the complicated structure of the lattice, which is shown in figure.



Crystal structure of BaY_2F_8.



Left panel: Decay of the integral RL signal intensity as a function of external magnetic field at applied 62 GHz microwaves.
Right panel: Angular dependences of the RL-EPR spectra. Simulation results are represented as curves, where the different colours correspond to two distinct centre orientations.

Recombination luminescence (RL) and RL-detected electron paramagnetic resonance (RL-EPR) in BaY_2F_8 single crystal has been investigated after irradiation with X-rays at low temperature. The recombination process, which lasts for several hours at 4 K, results in several broad bands in the RL spectrum. RL-EPR spectra show pronounced angular dependences on crystal orientation relative to external magnetic field. Based on the determined spin-Hamiltonian parameter values the recombination centres have been proposed to be F-type electron and self-trapped hole (V_K) centres.

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A.Antuzevics, A. Fedotovs, D. Berzins, U. Rogulis, K. Auzins, A. Zolotarjovs, S.L. Baldochi, J. Lumin. 223 (2020) 117216, doi: 10.1016/j.jlumin.2020.117216.

Portable low-cost open-source wireless spectrophotometer for fast and reliable measurements

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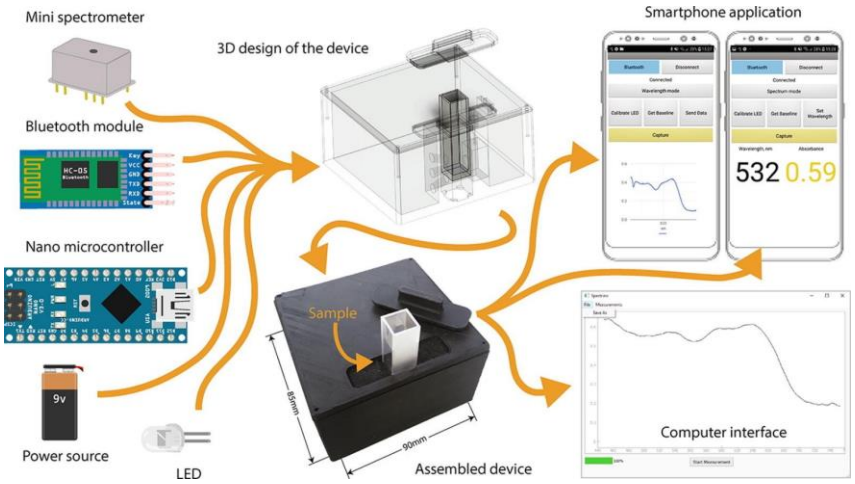
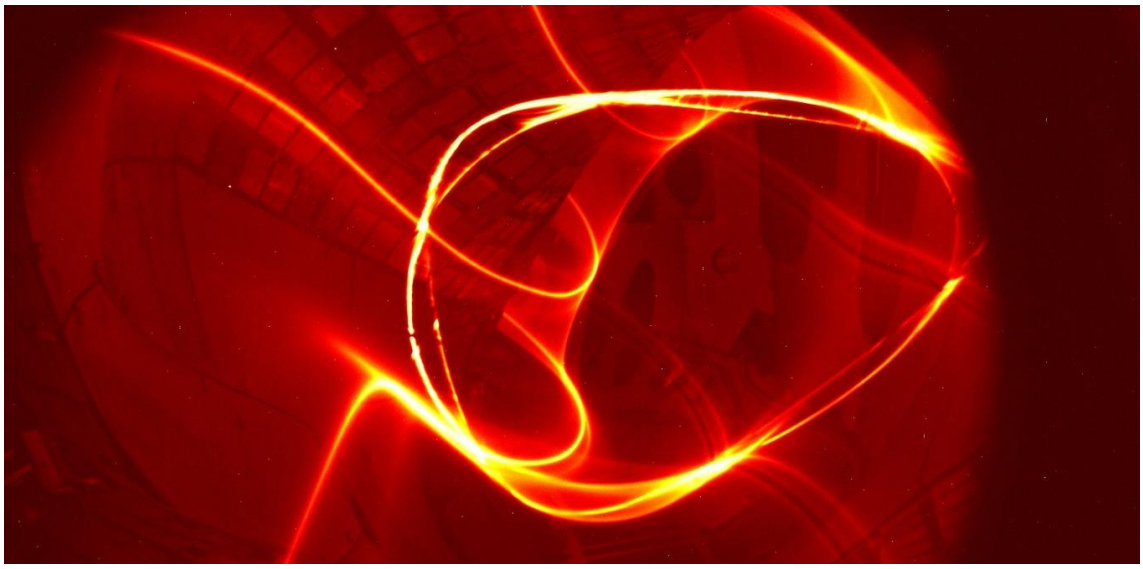
Spectrophotometric systems are widely used in studies across many fields such as physics, materials science, chemistry, biochemistry, biomolecular chemistry, photovoltaics and more. We demonstrate a low-cost standalone portable spectrophotometer for fast and reliable measurement execution. The data acquired can be both displayed via a dedicated smartphone application or a computer interface, allowing users either to gather and view data on the move or set up a continuous experiment. All design and software files are open-source and are intended for the device to be easily replicable and further customizable to suit specific applications. The assembled device can measure absorption in the wavelength range from 450 nm to 750 nm with a resolution of 15 nm and is housed in a 90 × 85 × 58 mm casing. Validation of the device was carried out by assessing wavelength accuracy, dynamic range and the signal-to-noise ratio of the system, followed by testing in three different applications where limit of quantification, limit of detection and relative standard deviations were determined. The results indicated better performance than low-cost spectrophotometers, on average being comparable to moderate to high-cost spectrophotometers.



The main components of the device – the mini-spectrometer, a Bluetooth module, nano microcontroller, an LED and a power source are featured on the left side. The 3D design and the assembled device can be seen in the middle of the figure and the smartphone application and the computer interface are on the right.

Published in:
K. Laganovska, A. Zolotarjovs, M. Vázquez, K. Mc Donnell, J. Liepins, H. Ben-Yoav, V. Karitans, K. Smits, HardwareX 7 (2020) e00108, doi: 10.1016/j.ohx.2020.e00108.

IV. Materials for energy harvesting and storage, clean energy transformation.



Influence of Nb-doping on the local structure and thermoelectric properties of transparent TiO_2:Nb thin films

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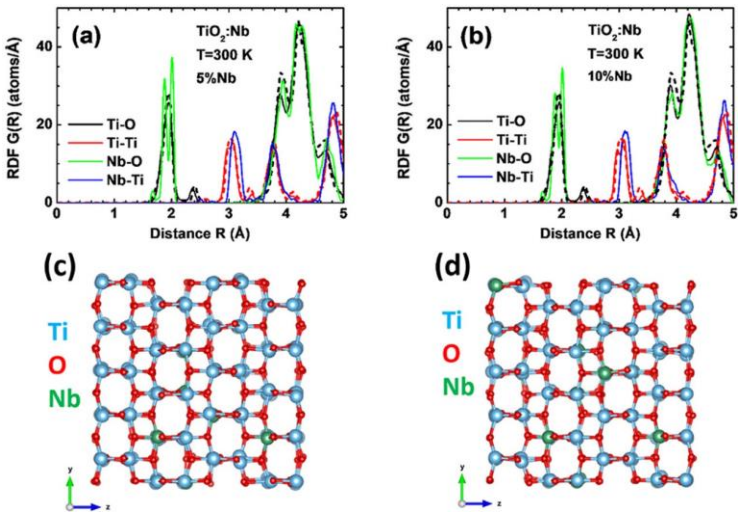
Transparent n-type niobium-doped titanium dioxide thin films (TiO_2:1.5at.%Nb) with pronounced thermoelectric properties were produced from a composite Ti:Nb target by reactive magnetron sputtering. The thin films were comprehensively characterized by X-ray diffraction, X-ray photoelectron spectroscopy, optical spectroscopy, electrical conductivity, and thermoelectric measurement techniques. The local structure of the thin films was investigated in detail by X-ray absorption spectroscopy at the Ti and Nb K-edges. A set of radial distribution functions were extracted from the simultaneous analysis of EXAFS data at two absorption edges using the reverse Monte Carlo method.

It was found that Nb dopant atoms modify the local environment of the films, but their average structure remains close to that of the anatase phase. This conclusion is also supported by the ab initio simulations of XANES. A very high absolute Seebeck coefficient (S= 155 mV/K) for n-type TiO_2 was achieved with Nb doping, yielding a maximum power factor and thermoelectric figure of merit of 0.5 $mWm^{-1}K^2$ and 0.18 at a temperature of 300 K, respectively, for a 150 nm thick film. From frequency-domain thermoreflectance experiments, a thermal conductivity value of 1.3 $Wm^{-1}K^2$ was obtained for the optimized TiO_2:Nb film.



Radial distribution functions (RDFs) G(R) calculated from the coordinates of atoms in a TiO_2 5 × 5 × 2 supercell at 300 K, for 5% and 10% of dopant Nb atoms. Dashed (black and red) curves are for RDFs *G*(Ti–O) and *G*(Ti–Ti) in anatase TiO_2 at T = 300 K. (c, d) Fragments of the RMC 5a × 5b × 2c supercells for c) 5% of Nb and d) 10% of Nb atoms.

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J.M. Ribeiro, F.C. Correia, A. Kuzmin, I. Jonane, M. Kong, A.R. Goni, J.S. Reparaz, A. Kalinko, E. Welter, C.J. Tavares, J. Alloys Compd. 838 (2020) 155561, doi:10.1016/j.jallcom.2020.155561.

Distinctive features of diffusion-controlled radiation defect recombination in stoichiometric magnesium aluminate spinel single crystals and transparent polycrystalline ceramics

A. Lushchik[a], E. Feldbach[a], E. A. Kotomin[b], I. Kudryavtseva[a], V. N. Kuzovkov[b], A. I. Popov[ab], V. Seeman[a], E. Shablonin[ab]

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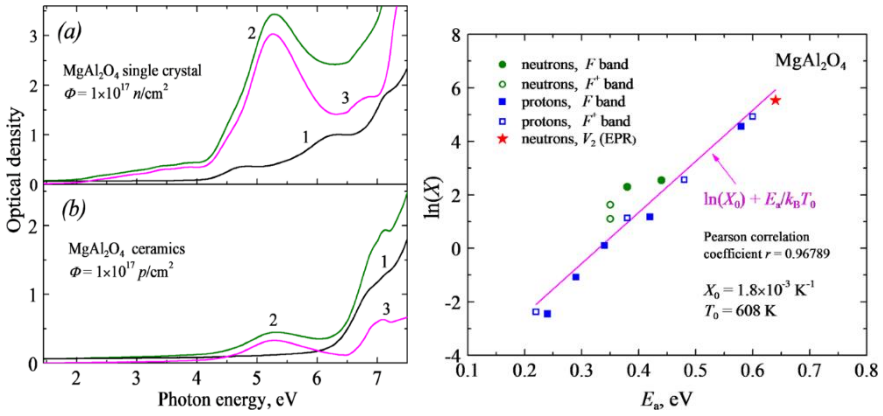
$MgAl_2O_4$ spinel is important optical material for harsh radiation environment and other important applications. The kinetics of thermal annealing of the basic electron *(F, F⁺)* and hole (*V*) centers in stoichiometric $MgAl_2O_4$ spinel irradiated by fast neutrons and protons is analyzed in terms of diffusion-controlled bimolecular reactions. Properties of $MgAl_2O_4$ single crystals and optical polycrystalline ceramics are compared. It is demonstrated that both transparent ceramics and single crystals, as well as different types of irradiation show qualitatively similar kinetics, but the effective migration energy Ea and pre-exponent D_0 are strongly correlated. Such correlation is discussed in terms of the so-called Meyer-Neldel rule known in chemical kinetics

$ln(X) = ln(X_0) + E_a/k_BT_0$

where X_0 is constant and T_0 characteristic temperature. Thus, the diffusion pre-exponent *X* turns out to be exponentially dependent on the migration energy. It is demonstrated that the involvement of both oxygen and cation interstitials is needed to describe the tentative scenario of the paramagnetic hole-containing centers in $MgAl_2O_4$ single crystal. A search for experimental manifestations of oxygen interstitials in $MgAl_2O_4$ (as well as in other binary and complex metal oxides) and the elucidation of their microstructure, preferable charge states, diffusion and trapping mechanisms still lies ahead.



Left panel: a) and b) The absorption spectra of an $MgAl_2O_4$ single crystal (a) or ceramic sample (b), grain size of 12 μm) measured at 295 K before (curves 1) and after irradiation with fast neutrons or 100-keV protons (curves 2). The difference spectra (curves 3) represent radiation-induced optical absorption (RIOA).
Right panel: Correlation of the effective migration energies Ea and pre-exponents X for radiation defect annealing in $MgAl_2O_4$.

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Atomic, electronic and magnetic structure of an oxygen interstitial in neutron-irradiated Al_2O_3 single crystals

V. Seeman[a], A. Lushchik[a], E. Shablonin[a,b], G. Prieditis[a], D. Gryaznov[b], A. Platonenko[b], E. A. Kotomin[b], A. I. Popov[a,b]

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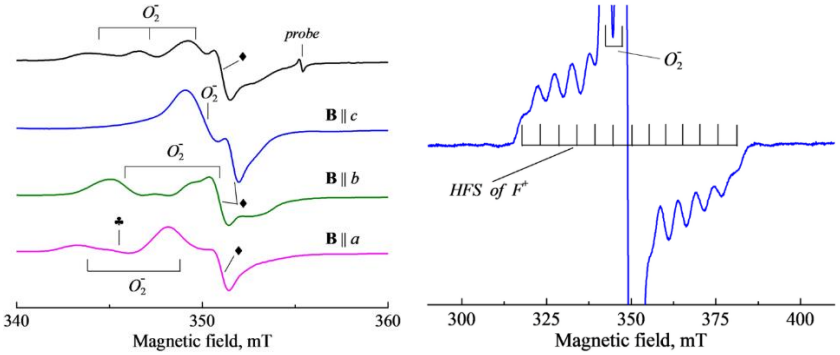
A single radiation-induced superoxide ion O_2^- has been observed for the first time in metal oxides. This structural defect has been revealed in fast-neutron-irradiated (6.9×10^{18} n/cm2) corundum (α-Al_2O_3) single crystals using the EPR method. Based on the angular dependence of the EPR lines at the magnetic field rotation in different planes and the determined g tensor components, it is shown that this hole-type O_2^- center (i) incorporates one regular and one interstitial oxygen atoms being stabilized by a trapped hole (S = 1/2), (ii) occupies one oxygen site in the (0001) plane being oriented along the a axis, and (iii) does not contain any other imperfection/defect in its immediate vicinity. The thermal stepwise annealing (observed via the EPR signal and corresponding optical absorption bands) of the O_2^- centers, caused by their destruction with release of a mobile ion (tentatively the oxygen ion with the formal charge −1), occurs at 500–750K, simultaneously with the partial decay of single *F*-type centers (mostly with the EPR-active F^+ centers). The obtained experimental results are in line with the superoxide defect configurations obtained via density functional theory (DFT) calculations employing the hybrid B3PW exchange-correlation functional. In particular, the DFT calculations confirm the O_2^- center spin S = 1/2, its orientation along the a axis. The O_2^- center is characterized by a short O–O bond length of 1.34 Å and different atomic charges and magnetic moments of the two oxygens. We emphasize the important role of atomic charges and magnetic moments analysis in order to identify the ground state configuration.



Left panel: EPR spectra measured at different orientation of B with respect to a, b and c axes of a neutron-irradiated α-Al_2O_3 crystal. The upper spectrum corresponds to ϕ = 16° between B and the axis a in the (0001) plane. Symbols (♣ and ♦) mark EPR signals of two unidentified radiation defects, signal of a test sample corresponds to g = 1.9800. T= 295K, P = 0.6mW.

Right panel: The F^+ center EPR spectrum for a neutron-irradiated Al_2O_3 crystal. P = 0.6 mW, RT, B⊥c and B//a (B lies in the (0001) plane).

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V. Seeman, A. Lushchik, E. Shablonin, G. Prieditis, D. Gryaznov, A. Platonenko, E. A. Kotomin, A. I. Popov, Sci. Rep. 10 (2020) 15852, doi:10.1038/s41598-020-72958-9.

Radiation-induced effects in neutron- and electron-irradiated lithium silicate ceramic breeder pebbles

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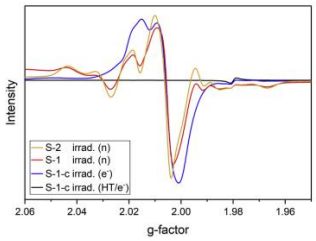
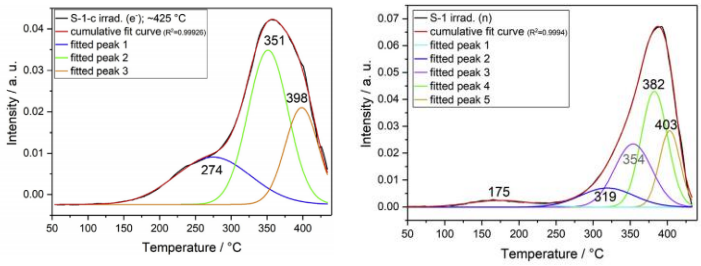
Ceramic breeder pebbles consisting of lithium orthosilicate (Li_4SiO_4) as the main phase and lithium metasilicate (Li_2SiO_3) as a secondary phase were analysed with respect to radiation-induced defects and radiolysis products. Therefore, pebbles that were irradiated with neutrons in the so-called HICU experiment (High neutron fluence irradiation of pebble stacks for fusion) were compared to pebbles irradiated with accelerated electrons. FTIR analysis revealed that Li_2SiO_3 band is more pronounced in neutron irradiation than electron irradiation as lithium transmutation to tritium takes place, but there were no significant changes or additional phases compared to accelerated electron-irradiated samples.

ESR (electron spin resonance) measurements revealed several paramagnetic radiation-induced defects and radiolysis products both for neutron and electron irradiation, such as E' centres, HC1 and HC2 centres, peroxide radicals, and either colloidal lithium particles or F^+ centres that were detected. Overall spectra are similar, and differences could be explained by low intensity after electron irradiation for specific centres. Radiation-induced defects and radiolysis products induced by neutron irradiation recover at relatively high temperatures of around 350 C because a partial recovery already happened during the irradiation. The thermal recovery in samples irradiated with neutrons at elevated temperatures can be described by electron-irradiated samples that are annealed after the irradiation. The obtained results for radiation-induced defects and radiolysis products suggest good comparability of neutron and accelerated electron irradiation if certain experimental parameters such as a low irradiation temperature and signals of very low intensity are considered during data processing.



ESR spectra of neutron-irradiated ceramics S1, S2 (n) and electron irradiated S1,(e) and S2 (HT/e) high temperature electron irradiation, where g=1.9800 is calibration marker.



Thermally stimulated luminesces glow curves for HT electron irradiated ceramics (left), and neutron-irradiated (right).

Published in:
J. M. Leys, A. Zarins, J. Cipa, L. Baumane, G. Kizane, R. Knitter, J. Nucl. Mater. 540 (2020) 152347, doi:10.1016/j.jnucmat.2020.152347.

First principles calculations of oxygen reduction reaction at fuel cell cathodes

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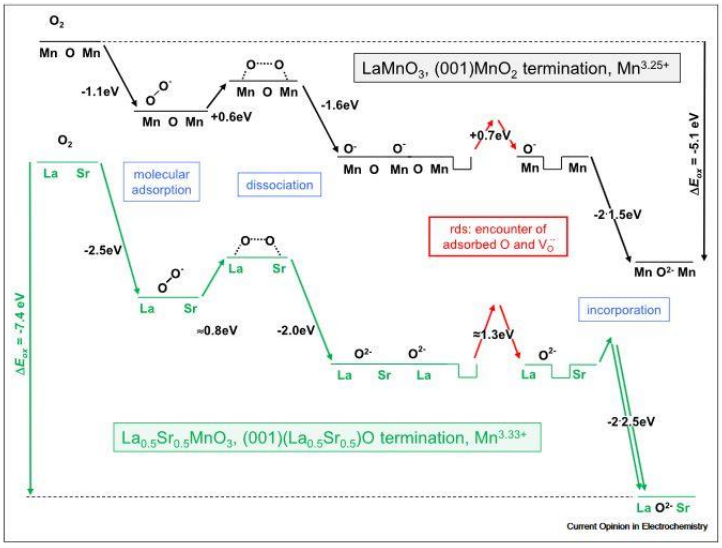
[b] *Max Planck Institute for Solid State Research, Stuttgart, Germany*

Solid oxide fuel cells (SOFC) allow for clean efficient conversion of chemical to electrical energy. The oxygen reduction reaction (ORR) is a multistep process that comprises molecular chemisorption, O-O bond dissociation, and incorporation of oxygen species into the surface of the fuel cell cathode material. Typically, one of these steps is much slower than the others and plays the role of the rate-determining step (rds), which defines the overall ORR rate. While certain information on the ORR mechanism and the rds can be extracted from experimental data, first principles calculations are an important complementary tool. They allow one to determine defect formation energies and migration barriers, which differ from bulk values, and supply transition state energies. For ABO_3 perovskites, low-index (001) AO and BO_2 surfaces typically represent the lowest energy terminations. The SOFC efficiency depends critically on materials, in particular for the cathode where ORR occurs. Typically, mixed conducting perovskite ABO_3-type materials are used for this purpose. The relative fractions of (001) AO and BO_2 surfaces depend on materials composition and ambient external conditions.



Here, results of recent large-scale first principles calculations for the two alternative polar (La,Sr)O and MnO_2(001) terminations of (La,Sr)MnO_3 cathode materials were discussed. The surface oxygen vacancy concentration for the (La,Sr)O termination is shown to be more than 5 orders of magnitude smaller compared to MnO_2, which leads to drastically decreased estimated ORR rates. Thus, it is predicted for prototypical SOFC cathode materials that the BO_2 termination largely determines the ORR kinetics, although with Sr surface segregation (long-term degradation) its fraction of the total surface area decreases, which slows down cathode kinetics.

Published in:
E. A. Kotomin, Yu. A. Mastrikov, R. Merkle, J. Maier, Current Opinion in Electrochemistry 19 (2020) 122-128, doi:10.1016/j.coelec.2019.11.005.

To the theory of gyrotrons with wide emitters

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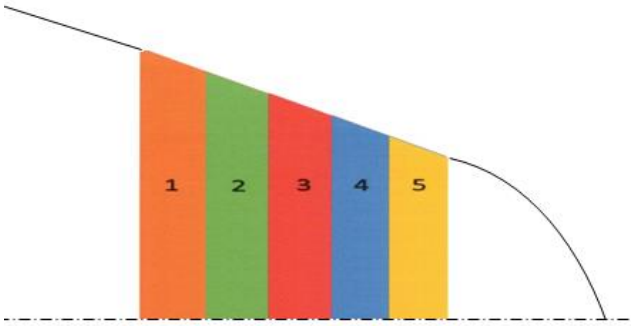
The main trends in gyrotron development are escalation of the radiated power and increasing the frequency of coherent radiation. For both trends it is beneficial to develop gyrotrons with wide emitters because this allows one to use cryomagnets with smaller inner bore sizes. For analyzing and optimizing the operation of gyrotrons with wide emitters it is proposed to represent such emitters as a superposition of thin rings and analyze the properties of electron beams emitted by each of these rings. The present paper consists of two parts. In the first part, the peak values of the orbital velocities and their spread are determined in all fractions of an electron beam in a gyrotron with the standard and widened emitters; also the effect of profiling the anode on characteristics of these electron beam fractions is considered. In the second part, the interaction efficiency of electron beams produced by thin emitter rings is described and the relationship between these efficiencies and orbital-to-axial velocity ratios in these beams is discussed.

Results obtained illustrate some advantages of characterizing gyrotron operation by considering the characteristics of electron fractions produced by thin layers of wide emitters. Of course, the widening of emitters, while allowing the development of more compact gyrotrons, also causes some negative consequences. One of them is the increase of the beam radial thickness that causes the efficiency degradation due to the radial nonuniformity of the transverse structure of the resonator mode.



Schematic representation of the emitter as a superposition of thin rings

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M. Proyavin, O. Dumbrajs, G. Nusinovich, and M. Glyavin, Journal of Infrared, Millimeter, and Terahertz Waves 41 (2020) 141, doi:10.1007/s10762-019-00646-5.

GYROCOMPU: Toolbox designed for the analysis of gyrotron resonators

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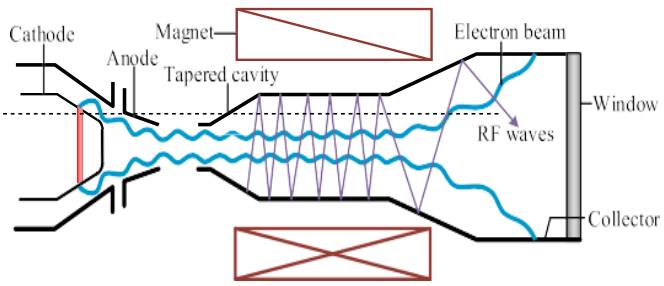
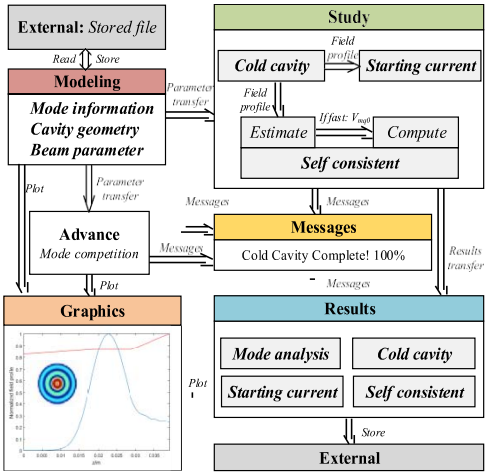
The key point of gyrotron design is the analysis of the radio frequency (RF) behavior in gyrotron resonators. This article proposes a comprehensive, user-friendly and effective gyrotron design toolbox (GYROCOMPU) based on the MATLAB platform. GYROCOMPU associates a relatively complete set of codes for gyrotron analysis and integrates them together into a graphical user interface (GUI). The solving algorithm of the cold cavity equations and self-consistent equations is improved. The solving method improvement in these calculation algorithms renders the analysis more efficient and accurate. Three typical examples of gyrotrons working in the 140-GHz TE_{03} mode, 42-GHz TE_{03} mode, and 140-GHz $TE_{10,4}$ mode are analyzed. All main codes, including the cold cavity calculation, starting current calculation, self-consistent calculation, and mode competition calculation, are compared with the classical code package (COAXIAL) or with results from the literature. The simulation results show that GYROCOMPU can accurately and effectively complete the analysis of gyrotrons.



Sectional view of a typical gyrotron



Architecture of GYROCOMPU

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P. Wang, X. Chen, H. Xiao, O. Dumbrajs, X. Qi, and L. Li, IEEE Transactions on Plasma Science 48 (2020) 11780-11789, doi: 10.1109/TPS.2020.3013299.

Interdependence of oxygenation and hydration in mixed-conducting (Ba,Sr)$FeO_{3-\delta}$ perovskites studied by density functional theory

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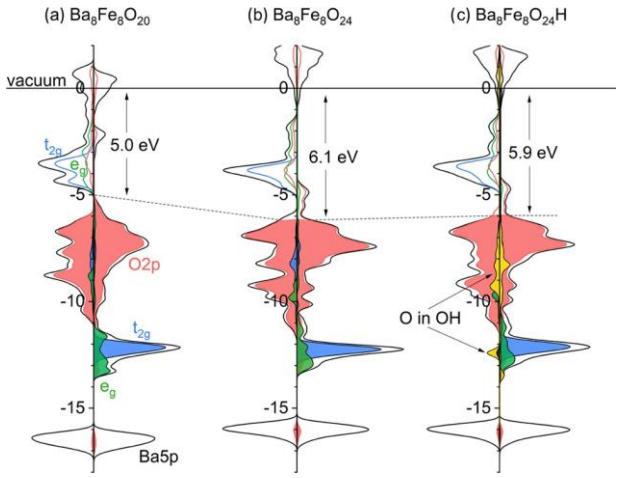
Protonic–electronic mixed-conducting perovskites are relevant as cathode materials for protonic ceramic fuel cells (PCFCs). The performance of PCFCs suitable for operation at intermediate temperatures of 400-600 °C has remarkably increased in recent years. This progress can be largely attributed to improvements in the material choice and fabrication of the proton-conducting perovskite solid solutions. So, proton-conducting electrolytes, typically $BaZr_{1-x}Y_xO_{3-x/2}$, were already intensively investigated. However, there is an urgent necessity to develop improved materials for the reduction of O_2 to water at the cathode. Optimized cathode materials with mixed protonic and electronic conductivity (e.g. (La,Ba,Sr)(Co,Fe,Zn,Y)$O_{3-\delta}$) are crucial for PCFC performance. However, they generally show lower degrees of hydration compared to the electrolyte. Therefore, (Ba,Sr)$FeO_{3-\delta}$ solid solutions are studied by using advanced density functional theory calculations, namely DFT+U approach, in order to get a deeper insight into the atomic and electronic structure.



Electronic density of states of fully oxidized (O24), reduced (O20), and protonated (O24H) $Ba_8Fe_8O_{24-\delta}H_x$ cells relative to a common vacuum level. O-in-OH states marked in yellow, are multiplied by a factor 4 for visibility. The dashed line indicates the position of Fermi energy.

We observe a nonideal dependence of the oxygen vacancies formation energy on δ for (Ba,Sr)$FeO_{3-\delta}$. It is attributed to the largely delocalized nature of oxygen holes. For the fully oxidized cell (O24 in figure) one can recognize empty O 2p states above the valence band maximum that correspond to the ligand hole at the O ions. Upon reduction (O20 in figure), these states become occupied, i.e. the Fermi energy shifts. Proton interstitials occupy a position close to oxygen, forming a covalent bond of the length of 0.97-1.01 Å. The formation of such bonds (024H in figure) leads to 1) stabilization in the energy of involved O 2p orbitals 2) a distinct deep state stemming the O 2p and H 1s overlap at -13 eV 3) a downward shift in the O 2p states of respective O ion that are not directly involved in the O-H bond. The calculated hydration energy spans a wide range (+0.2 - -1.0 eV depending on Sr content and δ). This highlights the importance of the redox activity of the oxide ions in these materials.

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M. F. Hoedl, D. Gryaznov, R. Merkle. E. A. Kotomin, J. Maier, J. Phys. Chem. C 124 (2020) 11780-11789, doi:10.1021/acs.jpcc.0c01924.

Proton, hydroxide ion, and oxide ion affinities of closed-shell oxides: importance for the hydration reaction and correlation to electronic structure

T. S. Bjørheim[a], M. F. Hoedl[b], R. Merkle[b], E. A. Kotomin[b,c], J. Maier[b]

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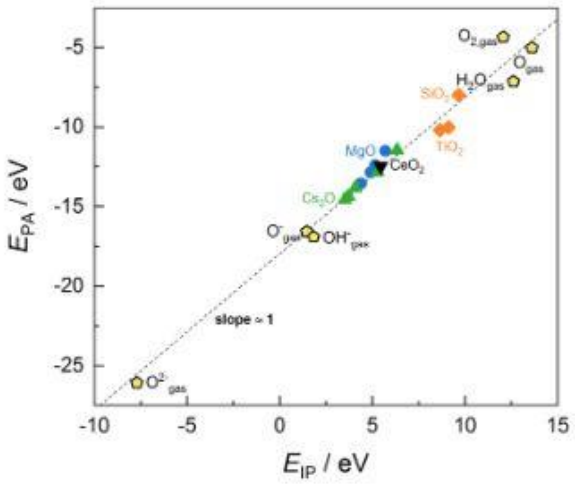
The interaction of water with metal-oxides is relevant in many research fields including geology, corrosion, catalysis, gas sensing, and energy conversion. While most oxides exhibit a rather high susceptibility for surface water adsorption and/or hydroxide formation, the propensity for water incorporation into the oxides' bulk varies greatly. A detailed understanding of the underlying mechanisms is of fundamental interest and is also important for the formation of mobile protonic carriers in fuel cells and membrane reactors. The dissociative water incorporation into oxides is a combination of protonation of regular oxide ions and hydroxylation of oxygen vacancies, typically introduced by acceptor doping.

Phenomenologically, the enthalpy of the dissociative water incorporation (hydration) of oxides is often found to be more favorable for more basic oxides. In the present work, we investigated proton, hydroxide ion, and oxide ion affinities (PA, HA, and OA) for 19 closed-shell oxides, ranging from Li_2O and Cs_2O to TiO_2, SnO_2, and SiO_2, including also ABO_3 perovskites, such as $SrTiO_3$ and $BaZrO_3$ using advanced first- principles defect calculations and thermochemical cycles. The proton affinity is found to play a predominant role in hydration thermodynamics. The ion affinities are strongly correlated with the oxides' electronic structure (specifically, the ionization potential (IP)). This intriguing correlation between PA and IP holds also for gaseous O species, suggesting a very general origin. Understanding the major factors controlling a metal oxide susceptibility for dissociative hydration of oxygen vacancies is not only of fundamental interest but also key to the successful development of novel mixed proton−electron conducting oxides for protonic ceramic fuel and electrolyzer cells.



Proton affinity of binary oxides as a function of the ionization potential

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T. S. Bjørheim, M. F. Hoedl, R.Merkle, E. A. Kotomin, J. Maier, J .Phys. Chem. C 124 (2020) 1277-1284, doi:10.1021/acs.jpcc.9b07570.

Time resolved luminescence spectroscopy of $CsPbBr_3$ single crystal

M. Dendebera[a], Ya Chornodolskyy[a], R. Gamernyk[a], O. Antonyak[a], I. Pashuk[a], S. Myagkota[b], I. Gnilitskyi[c,d], V. Pankratov[e], V. Vistovskyy[a], V. Mykhaylyk[f], M. Grinberg[g], A. Voloshinovskii[a]

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[b] *Lviv State Agrarian University, 1 V. Velykyi Str., Dublyany, Ukraine*
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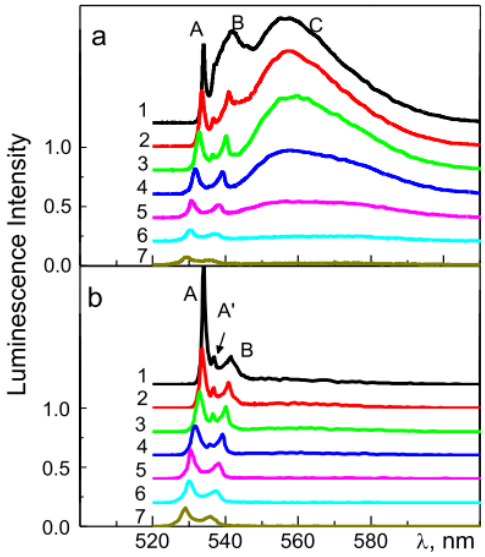
Within the family of halide perovskites $CsPbBr_3$ attracts special attention because of favourable physical and chemical characteristics as well as its stability at ambient conditions and relative easiness of production. Bulk $CsPbBr_3$ exhibit intense luminescence only at low temperatures that can explain lack of interest to the investigation of luminescence properties of $CsPbBr_3$ single crystals. This motivated us to study luminescence and kinetic parameters of $CsPbBr_3$ single crystals in 12–90 K temperature range in order to identify the structure of excitonic energy states involved in the luminescence processes.

Narrow luminescence bands at 534, 537, and 541.5 nm were detected at low temperatures using time-resolved luminescence spec-troscopy. They can be interpreted as follows. The first two bands can be attributed to the emission of free exciton and excitonic phonon replica. The nature of 541.5 nm band is discussed and, in many cases, inter-preted as the emission of bound exciton. The recombination character of this luminescence band at T >60 K poses a problem for such interpre-tation. Therefore, assignment of this band to indirect transitions from Rashba minima of conduction band can be more promising. Observed fast and slow luminescence components for 534 and 541.5 nm bands may be associated with the splitting of radiative states due to the exchange interaction. For the long-lived luminescence in 560 nm region, three broad emission bands were detected with peaks at 572, 556, and 541.5 nm and quenching energies of 38, 13, and 4 meV, respectively. It is assumed that these bands can be attributed to the luminescence of excitons trapped on the lattice defects or the luminescence of donor-acceptor pairs.



Luminescence spectra of $CsPbBr_3$ crystal measured in integral mode (a) and time window 5 ns (b) at 14 (1), 21 (2), 30 (3), 40 (4), 50 (5), 60 (6) and 70 K (7).

Published in:
M. Dendebera, Ya Chornodolskyy, R. Gamernyk, O. Antonyak, I. Pashuk, S. Myagkota, I. Gnilitskyi, V. Pankratov, V. Vistovskyy, V. Mykhaylyk, M. Grinberg, A. Voloshinovskii, J. Lumin. 225 (2020) 117346, doi: 10.1016/j.jlumin.2020.117346.

Matching the directions of electric fields from triboelectric and ferroelectric charges in nanogenerator devices for boosted performance

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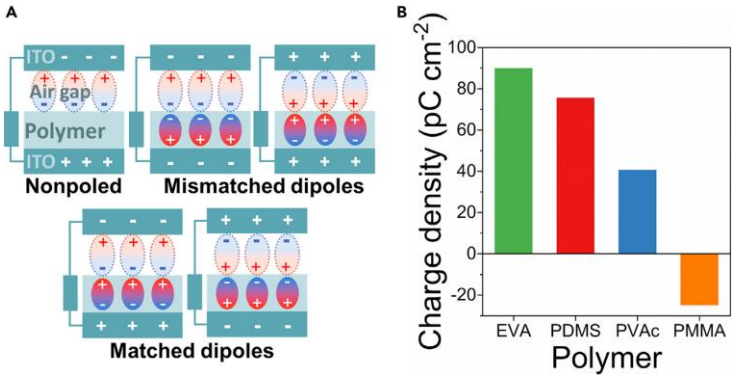
The field related to triboelectric nanogenerator (TENG) devices is emerging rapidly. The working principle of TENG devices is straightforward. The triboelectric materials (most commonly polymer insulators) are deposited on two conductive electrodes connected by an external circuit. Upon contacting-separating or sliding, surface charges are formed on the triboelectric materials, which induce an electrostatic charge on the conductive electrodes. Due to electrode oscillation or movement, a potential difference is created, which causes a current flow in the external electric circuit.

Embedding additional ferroelectric dipoles in contacting polymer layers is known to enhance the performance of triboelectric nanogenerator (TENG) devices. However, the influence of dipoles formed between the triboelectric surface charges on two contacting ferroelectric films has been ignored in all relevant studies. We demonstrate that proper attention to the alignment of the distinct dipoles present between two contacting surfaces and in composite polymer/$BaTiO_3$ ferroelectric films can lead to up to four times higher energy and power density output compared with cases when dipole arrangement is mismatched. For example, TENG device based on PVAc/$BaTiO_3$ shows an energy density increase from 32.4 μJm^{-2} to 132.9 μJm^{-2} when comparing devices with matched and mismatched dipoles. The presented strategy and understanding of resulting stronger electrostatic induction in the contacting layers enable the development of TENG devices with greatly enhanced properties. TENG devices can be integrated into fabrics, wearables, interior objects, membranes, and even implantable devices.



Dipole formed between polymer and ITO can be matched with ferroelectric dipole. Schematic representation of possible interactions between surface charge dipoles in the air gap and ferroelectric dipoles in TENG device (A). The calculated surface charge density of non-ferroelectric polymers indicates the magnitude and direction of the formed dipole in the contact-separation cycle (B).

Published in:
A. Šutka, K. Mālnieks, L. Lapčinskis, M. Timusk, K. Pudzs, M. Rutkis, iScience 23 (2020) 101011, doi: 10.1016/j.isci.2020.101011.

Theses

Doctoral Theses

No.	Author	Title	Supervisor	Degree
1.	**Aleksejs Gopejenko**	First Principles Simulations on Yttrium and Oxygen Precipitation Inside Fcc-Fe Lattice	Dr. chem. **Yuri Zhukovskii**	Dr.phys.
2.	**Edgars Butanovs**	Synthesis and properties of core-shell nanowires containing transition metal chalcogenides	Dr.phys. **Boris Polyakov**	Dr.phys.
3.	**Guna Krieķe**	Erbium upconversion luminescence in transparent glass ceramics containing ternary fluoride nanocrystals	Dr.phys. **Anatolijs Šarakovskis**	Dr.phys.
4.	**Arturs Bundulis**	Inquiry of the Kerr effect origins in organic materials: experimental assessment by Z-scan method	Dr.phys. **Mārtiņš Rutkis**	Dr.phys.

M.Sc. Theses

No.	Author	Title	Supervisor	Study programme
1.	**Anna Ivanova**	Catalytic activity of graphen electrode in the electroxidation of water to H_2O_2: modeling from the first principles	Dr.phys. **Sergejs Piskunovs**	Chemistry
2.	**Dāvis Zavickis**	Calculations of cobalt and iron-containing perovskite materials using the LCAO method with hybrid density functionals	Dr.rer.nat. **Guntars Zvejnieks**	Physics
3.	**Līga Bikše**	Structure and chemical composition of solid solutions based on $Na_{0.5}Bi_{0.5}TiO_3$	Dr.phys. **Ēriks Birks**	Physics
4.	**Dainis Bošs**	Legal aspects of hydrogen implementation procedure	Dr.phys. **Jānis Kleperis**	Social sciences

B.Sc. Theses

No.	Author	Title	Supervisor	Study programme
1.	**Patrīcija Paulsone**	Investigations of light amplification properties of new synthesis glass-forming pyranilidene derivatives	Dr.phys. **Aivars Vembris**	Physics
2.	**Oskars Bitmets**	Obtaining PEDOT-containing nanofibers by electrospinning method and characterization of their electrical properties	Dr.phys. **Kaspars Pudžs**	Physics
3.	**Reinis Kaparkalējs**	Osmosis phenomenon in sulfonated polyetheretherketone and zirconia composite membranes in $KHCO_3$ solution	Asoc.prof. Dr.chem. **Guntars Vaivars**	Chemistry
4.	**Ināra Ņesterova**	Synthesis and electrochemical properties of $Na_2FeP_2O_7/C$	Dr.phys. **Gints Kučinskis**	Chemistry
5.	**Aija Kalniņa**	Persistent luminescence of divalent manganese doped magnesium germanate material	Dr.phys. **Guna Doķe**	Physics
6.	**Čiro Frederiko Tipaldi**	Lattice dynamics calculations for $Mg_xZn_{1-x}O$ solid solutions	Dr.phys. **Jevgēņijs Gabrusenoks**	Physics
7.	**Haralds Ozols**	Superhyperfine structure of electron paramagnetic resonance spectra in chromium-activated lanthanum oxychloride	Dr.phys. **Andris Antuzevičs**	Physics
8.	**Viktorija Pankratova**	Investigation of luminescence properties of coactivated $Gd_3(Ga,Al)_5O_{12}$:Ce crystals	Dr.phys. **Anatolijs Šarakovskis**	Chemistry
9.	**Rihards Ruska**	Red and infrared luminescence in wide band gap materials	Dr.habil.phys. **Baiba Bērziņa**	Physics
10.	**Kaspars Vītols**	Europium ion photoluminescence in silver nanoparticle-containing oxyfluoride glass-ceramics	MSc. **Meldra Ķemere**	Physics

Other important news

Photo: Ilmārs Znotiņš, Office of the President

Achievements

- L`ORÉAL Baltic "For Women in Science" award given to researcher from ISSP UL's Laboratory of Optical Materials **M.Sc.Chem. Ivita Bite** for her research analyzing different chemical synthesis methods on the morphological and physical properties of materials such as intrinsic defects and optical properties.

https://www.facebook.com/lorealbaltics/videos/827156381490022

- Within the framework of Science Excellence and Commercialization support program of University of Latvia (UL), authors of the most outstanding publications within UL in 2019 have been awarded. Their publications correspond to Web of Science Q1 level. Among them also leading researcher from the ISSP UL's Laboratory of Visual Perception **Dr.phys. Varis Karitāns**, who received recognition for his article "Optical phase retrieval using four rotated versions of a single binary amplitude modulating mask" (published in Journal of Astronomical Telescopes Instruments and Systems)**.**

https://www.spiedigitallibrary.org/journals/Journal-of-Astronomical-Telescopes-Instruments-and-Systems/volume-5/issue-3/039004/Optical-phase-retrieval-using-four-rotated-versions-of-a-single/10.1117/1.JATIS.5.3.039004.short?SSO=1

- Lecturer of Physics department of UL Faculty of Physics, Mathematics and Optometry (FPMO) and leading researcher of ISSP UL's Spectroscopy laboratory **Dr.phys. Andris Antuzevičs** received the best UL lecturer award. Every year, the Mobility department of UL student service carries out a survey of foreign students, in which they evaluate their study experience in UL.

- Baltic Assembly Prize in Science was awarded to ISSP UL's leading researcher in Laboratory of Computer Modeling of Electronic Structures of Solids **Dr.phys. Roberts Eglītis** for his research cycle "Theoretical predictions for new materials for energy storage and harvesting".

https://www.saeima.lv/en/news/saeima-news/29218-the-baltic-assembly-prize-in-science-to-be-awarded-to-physicist-roberts-eglitis

- The senate of Latvian Academy of Sciences (LAS) awarded leading researcher of ISSP UL **Dr.phys. Jānis Kleperis** with Artūrs Balklavs prize for merit in popularizing science by organizing "Solar Cup" competition, which introduces school youth to alternative energy sources and their use. LAS name awards received by the following ISSP UL researchers - Edgars Siliņš Award in Physics - **Dr.phys. Aleksejs Kuzmins**; Ludvigs and Māris Jansons Award in Physics – **Dr.phys. Kaspars Pudžs**. LAS Young scientist award – **Dr.phys. Virgīnija Vītola**.

https://www.camart2.com/en/news/latvian-academy-of-science-lza-presents-name-and-young-scientists-awards.html

- LAS has recognized research "In-depth understanding of the functional properties of modern materials under extreme radiation conditions and their prediction" conducted by the ISSP UL's researchers Dr.phys. **A. Popovs**, Dr.habil.phys. **V. Kuzovkov**, Dr.habil.phys. **J. Kotomin**, Dr.rer.nat. **D. Grjaznov**, Mg. **A. Platoņenko** un PhD **E. Shablonin** and prof. A. Luschik from Institute of Physics, University of Tartu as one of the most significant achievements in Latvian science in 2020. https://www.cfi.lu.lv/en/about-us/news/detailed-view/t/63553/

- LAS President's Letter of Commendation received by ISSP UL's Dr. phys. **Varis Karitāns**, Dr. phys. **Sergejs Fomins**, Dr. habil. phys. **Māris Ozoliņš**, MSc. **Katrīna Laganovska**, MSc. **Kārlis Kundziņš** for their work "New optical and mathematical methods to improve image quality".

- LAS President's Letter of Commendation receivers from ISSP UL Mg. phys. **Natālija Tetervenoka** and Dr.phys. **Aivars Vembris** for participation in research **"New synthetic methods in purine chemistry and their application in materials science", conducted together with** scientists from the Faculty of Material Science and Applied Chemistry of RTU and of Latvian Institute of Organic Synthesis.

https://www.camart2.com/en/news/researches-carried-out-at-issp-ul-among-most-significant-achievements-in-latvian-science-in-2020-named-by-latvian-academy-of-sciences.html

- On November 26, during the LAS general meeting and elections by the secret ballot, the leading researcher of ISSP UL Dr.phys. Roberts Egītis was elected as true member of LAS and leading researcher and Deputy Director for Science of the ISSP UL Dr.hab.phys. Andris Šternbergs was elected as vice-president of the LAS.

Conferences and events organized by ISSP

- February 7–9. ISSP UL organized **Deep Science Hackathon** in which the strongest materials based and technological ideas and teams with innovation potential took part. Participants represented India, Denmark, Lithuania, Nepal and Latvia.
- February 11-13. **36th scientific conference of ISSP UL** took place. 28 oral and 47 poster presentations were given. 55% of the speakers were students or young scientists.
- February 27, ISSP UL held administrative meeting of **EURO*fusion* research project** "Advanced experimental and theoretical analysis of defect evolution and structural disordering in optical and dielectric materials for fusion applications" - **AETA** (Advanced experimental and theoretical analysis of defect evolution and structural disordering in optical and dielectric materials for fusion applications) to evaluate the achieved progress and plan next steps for the successful completion of the project.
- February 27 – first **ISSP UL's "Scientists' breakfast"** took place. Dr.phys. Andris Anspoks ISSP UL's Deputy Director for Innovation discussed the new science program, its structure, content and challenges.
- March 12, the opening of the **Taiwan and Baltic Physics Research Center** took place at ISSP UL. Its aim is to ensure exchange visits of students, leading researchers and professors, use of ISSP UL open access laboratory equipment, as well as organization of mutual educational seminars on the latest research methods and results. The opening of the center was attended by scientists and government representatives from Taiwan's National Sun Yat-sen University, the University of Latvia, as well as guests from the Saeima, UNESCO, the State Education Development Agency and the Ministry of Foreign Affairs of Latvia.
- March 26, second **ISSP UL's "Scientists' breakfast"** took place. Head of Laboratory of Materials for Energy Harvesting and Storage Dr. phys. Gints Kučinskis spoke about current challenges and research on lithium ion batteries.
- April 30, third **ISSP UL's "Scientists' breakfast".** Theme – cooperation with RISE/KTH in science and research. For instance, ISSP UL's cooperation with RISE on application of CQD and CNP photonic sensors in forensics (detection of controlled substances).
- May 28, **ISSP UL's "Scientists' breakfast".** Head of Laboratory of Prototyping of Electronic and Photonic devices Dr.sc.ing Gatis Mozoļevskis told about two new pieces of equipment – electron beam lithography equipment (in cleanrooms) and atomic layer deposition equipment.

Head of Materials Morphology and Structural Investigations Dr.phys. Krišjānis Šmits – about new SEM microscope.

- September 29, **ISSP UL's "Scientists' breakfast".** Theme – commercialization projects of Investment and Development Agency of Latvia. Leaders of the institute teams currently implementing one of these projects shared their experience and recommendations.
- October 16-18. ISSP UL held second **Student Deep Science Hackathon**. The event took place online and gave students the opportunity to develop their innovative ideas in a virtual workshop and meet like-minded people and form interdisciplinary teams with innovation potential.
- October 29. Another **ISSP UL's "Scientists' breakfast"** took place. This time guests were scientists Vjačeslavs Kaščejevs and Andris Ambainis, who discussed the National Research Program in quantum technologies in which ISSP UL plays and important role.

Scientific projects

- In 2020 ISSP UL implemented 67 projects:

International:

- two HORIZON 2020 projects;
- three EURO*fusion* projects;
- three COST projects;
- two EraNet projects;
- one Latvia-France bilateral cooperation project OSMOZE;
- one Latvian-Ukrainian bilateral cooperation program;
- two Latvia-Lithuania-Taiwan trilateral cooperation projects;

National:

- one National Research Program (NRP) project;
- one EAFRD project;
- eighteen ERDF projects;
- twenty one Latvian Council of Sciences projects;
- ten postdoctoral projects;
- two Rural support service projects;

- In a competition of Fundamental and Applied Research projects, 4 projects submitted by ISSP UL were accepted.
- In NRP "Mitigation of Covid-19 effects", two sub-projects supervised by researchers of ISSP UL were approved.

Participation in conferences

- In 2020, ISSP UL's researchers participated in more than 15 scientific conferences and seminars with more than 60 oral/poster presentations. Due to Covid-19 travel restrictions, these events mostly took place online.
- January 21-24, leading researchers from ISSP UL's Laboratory of Kinetics in Self-organizing Systems Dr.habil.phys. Eugene Kotomin and Dr.rer.nat. Yuri Mastrikov participated in conference "**Electronic Materials and Applications EMA-2020"**.
- January 31- February 6, Head of Laboratory of Prototyping of Electronic and Photonic devices Dr.sc.ing Gatis Mozoļevskis participated at **"SPIE Photonics West"**.

• February 20-21. Head of ISSP UL's EXAFS Spectroscopy Laboratory Dr.phys. Alexei Kuzmin with invited speech participated at **1st PanPacific Reverse Monte Carlo Conference**.

• October 19-23, researchers from ISSP UL's Thin Films Laboratory Dr.phys. Boris Polyakov and MSc. Edgars Butanovs participated at **"Graphene 2020"** conference.

• November 23-26, researchers from ISSP UL participated at the **International Scientific Conference FM&NT**. This year 17 countries were represented in the virtual conference – among them Latvia, Lithuania, Ukraine, Russia and Estonia stood out with the largest number of participants.

Attracting young scientists

• In the regular competition for ISSP UL's Students and Young Scientists grants from Institute's financial reference amount were allocated to the master's degree students **Ernests Einbergs**, **Miks Krišjānis Jurjāns**, **Madara Leimane**, **Viktorija Pankratova**, doctoral students - **Kevon Kadiwala**, **Kaspars Kaprāns**, **Pēteris Lesničenoks** and young scientist **Raitis Gržibovskis**.

• 8 projects have won postdoctoral research competition – Dr. **Thomas Yager**, Dr. **Arūnas Strike**, Dr. **Zarina Umatova**, Dr. **Mārtiņš Zubkins**, Dr. **Rakesh Saroha**, Dr. **Sudeshna Samanta**, Dr. **Anna Pidluzhna**, Dr. **Andrejs Ogurcovs**.

• Gratuities payed for successfully developed and defended qualification works as well as for highest performance ratios in 2020 among groups of researchers' assistants, researchers, leading researchers and heads of laboratories.

• Extra payments from the financial reference amount allocated to students starting to work at the institute.

•

Other activities

• January 30. The Bank of Latvia organized experts talks **"From money acquisition to smart investment"** – how to invest wisely the European Union's funds to increase long-term prosperity in Latvia. ISSP UL's Deputy Director for Innovation Dr.phys. Andris Anspoks participated in the event and emphasized the importance of developing STEM education and not direct all the most capable pupils to the IT field, because lack of students in physics, chemistry, and biology is observed which does not allow maintaining the engineering skills at high level in the country.

• In January, EC's 9th framework program or Horizon Europe EURO*fusion* "Enabling Research Activities" organization has appointed members of Scientific board responsible for evaluation of project applications, identification of projects to be funded and evaluation of scientific results. ISSP UL's leading researcher from Laboratory of Kinetics in Self-organizing Systems Dr. phys. Anatoli Popov was appointed member of materials branch of EURO*fusion* Enabling Research Activities projects board.

• In January and February ISSP UL's Deputy Director for Innovation Dr.phys. Andris Anspoks participated in two EuroNanoLab consortium meetings.

• On February 6, ISSP UL's project manager Juris Kļava participated in a radio program "Kā labāk dzīvot" (*How to live better*) on **Latvian Radio 1 (LR1)**. Theme of the program "Hackathon – opportunity to implement ideas in important projects". He explained what a hackathon is and how ideas are turned into significant projects.

https://lr1.lsm.lv/lv/raksts/ka-labak-dziivot/hakatons-iespeja-savas-idejas-istenot-nozimigos-projektos.a126215/

• On February 6, ISSP UL's leading researcher Marija Dunce was a guest in **LR1** program "**Zināmais nezināmajā**" (*Known in the unknown*). Scientists around the world are looking for ways to create materials that could replace lead or more specifically lead zirconate titnate in different technologies. Such research is also taking place in Latvia – at ISSP UL. https://lr1.lsm.lv/lv/raksts/zinamais-nezinamaja/jauni-materiali-svina-aizstasanai.-latvijas-zinatnieku-petijumi.a126217/

• On February 12, **Job Shadow Day** organized by Junior Achievement career education program for students of grades 1-12 took place during which school students attended chosen work place and observed the everyday work life of a representative of chosen profession. 16 pupils aged 12-19 from different parts of Latvia came to see how ISSP UL's scientists work. Within the Job Shadow Day activities, deputies of European Affairs Committee of the Saeima of Latvia wanted to inform their job shadows about the good examples of attracting the EU financing and invited ISSP UL's director Dr.phys Mārtiņš Rutkis to tell about CAMART^2 project, work and development of ISSP UL. Whereas Deputy Director for Education of the ISSP UL Dr.phys. Anatolijs Šarakovskis informed about Institute's contribution to the development of the education program.

• On Ferbuary 13, filming team of **EuroNews *Futuris*** program visited ISSP UL with the aim to make a story about, in their opinion, best of the Horizon Teaming projects. The material was broadcasted on EuroNews channel 22 times from March 9-13. EuroNews broadcasts its programs in 130 countries, 12 languages and its audience is 430 million viewers.

https://www.euronews.com/2020/03/09/eu-funding-dramatically-changing-innovation-in-latvia

• February 27. EURO*fusion* ATEA project meeting was held at ISSP UL as well as MASOC cluster/members external meeting took place at the ISSP UL.

• On March 5 in an **online journal NORDISCH.info** an article about LAS most significant Latvian scientific achievement in 2019 - "Theoretical predictions for new materials for energy storage and harvesting" by ISSP UL's researchers Dr.phys. Roberts Eglītis, Dr.habil.phys. Juris Purāns, Dr.phys. Jānis Kleperis and Dr.phys. Anatolijs Popovs was published.

https://www.nordisch.info/lettland/wissenschaftler-entwickeln-bessere-batterien/

• On March 6, the **president of the Republic of Latvia Egils Levits** visited the ISSP UL. J. Kažociņš – adviser on national security, A. Pīka – adviser on economic policy, I. Siliņa – external adviser on education and science, R. Lappuķe – external adviser on smart technologies and S. Ēlerte – adviser on cultural policy also took part in the visit.

https://www.president.lv/lv/jaunumi/zinas/valsts-prezidents-izsaka-gandarijumu-par-lu-cietvielu-fizikas-instituta-devumu-latvijai-un-pasaulei-26169#gsc.tab=0

• In April ISSP UL became a member of **EPIC** (European Photonics Industry Consortium).

• On April 22, innovation and technology platform **Labs of Latvia** published information and interview with ISSP UL's Deputy Director for Innovation Dr.phys. Andris Anspoks about ISSP UL as an important center of excellence in the Baltic States in education, science, innovation and technology transfer as well as about success achieved thanks to CAMART^2 project. https://labsoflatvia.com/aktuali/cfi-starptautiski-projekti

• On May 12 seminar organized by Latvian Council of Science about Fundamental and Applied Research projects in natural sciences. ISSP UL's researchers– Deniss Grjaznovs, Anatoli Popov, Linards Skuja, Uldis Rogulis and Laima Trinklere told about their research.

- On May 28 at the center of attention in Latvian National TV program **"Izziņas impulss"** (*Quest impulse*) was physics. Head of the Laboratory of Prototyping of Electronic and Photonic Devices Dr.sc.ing. Gatis Mozoļevskis was the guest in the program.
- On May 27, RīgaTV24 broadcasted program **"Izvēlies panākumus!"** (*Choose success*)**.** Head of Laboratory of Optical Materials of ISSP UL Dr.phys. Virgīnija Vītola told about FPMO of the UL, keys to success and work of the scientist.

https://xtv.lv/rigatv24/video/6M5GnnMbGoz-27_05_2020_izvelies_panakumus_2_dala

- On June 3, "Delfi Campus" article about video program **AlmaMater.lv** in which one of the heroes was ISSP UL's scientist Marija Dunce.

https://www.delfi.lv/campus/raksti/zinatniekam-noder-ari-laba-intuicija-divu-fiziku-portreti-raidijuma-alma-mater?id=52193433

- On July 2, this year's L`ORÉAL Baltic "For Women in Science" award winners made guest appearances in LR1 program **"Zināmais nezināmajā"** (*Known in the Unknown*)**.** One of them was ISSP UL's researcher from the Laboratory of Optical Materials M.Sc.Chem. Ivita Bite.

https://lr1.lsm.lv/lv/raksts/zinamais-nezinamaja/loeral-baltic-programmas-sievietem-zinatne-laureates-no-latvijas.a131710/

- On August 4, **UL Foundation** homepage and on August 24 "**Delfi Campus**" published an article about ISSP UL's researcher from EXAFS Spectroscopy Laboratory "Passionate PhD student Inga Pudža studies the structure of materials and in laboratory feels like a fish in the water". https://www.fonds.lv/par-mums/zinas/zina/t/60320/
- On September 3, the new director of the **Latvian Council of Science (LCS) Gita Rēvalde** visited the ISSP UL. The aim of the visit was to discuss the strategy of the newly established LCS and the possibilities of cooperation with the institute as well as to see the renovated laboratories and get acquainted with the infrastructure.
- On September 8, in a seminar "Different types of technology companies and opportunities in them" organized by **Riga TechGirls education program**, Inga Pudža told about ISSP UL, herself and her work at the EXAFS Spectroscopy Laboratory.
- On September 22, the **Minister of Education and Science of the Republic of Latvia Ilga Šulpinska** visited ISSP UL. The minister was accompanied by Dmitrijs Stepanovs, Deputy Secretary of State for Higher Education, Science and Innovation. They were acquainted with the institute, visited cleanrooms and discussed academic cooperation, financial reference amount, opportunities of ISSP UL with the researchers as well as the development of science and higher education in the future.
- On September 25, the closing event of the UL New Technologies and Innovation Days took place during which **"Knowledge Agora"** event was organized. At the event, UL researchers and students presented their research. From ISSP UL researcher from Laboratory of Materials for Energy Harvesting and Storage Pēteris Lesničenoks told about WILEG (Innovative Wave Energy Converter, Linear Electric Generator) project.
- On September 29, **Ivars Ijabs, member of the Europeam Parliament** and his assistant Pēteris Viņķelis visited the ISSP UL. The purpose of the visit was to see the institute, which is No 1 according to the amount of EC funding in Latvia, see the renovated laboratories and get to know about the research performed at the institute.
- On October 27-29, ISSP UL's researchers participated in international hackathon **"Photon and Neutron Science in the Baltic Sea region"**.

- On November 5, at **India Nordic Baltic Conclave** (India-NB8) ISSP UL was represented by Head of the Laboratory of Materials for Energy Harvesting and Storage Dr.phys. Gints Kučinskis and Head of the Laboratory of Chemical Technologies Asoc.prof.Dr.chem. Guntars Vaivars.
- On November 10, on the World Science Day for Peace and Development, ISSP UL's researcher Dr.phys. Līga Grīnberga was a guest at the UL's **"Science Cafe".** Theme of the event – "Women in science – dare to achieve".
- On November 12, on LTV1 program **Rīta Panorāma** (*Morning Panorama*) there was a news story about the gallium oxide research performed at the ISSP UL and together with the Swedish colleagues and the role of gallium oxide in the fight against SARS-CoV-2.

https://ltv.lsm.lv/lv/raksts/12.11.2020-gallija-oksids-varetu-palidzet-cina-ar-virusiem.id201982/

- November 13-14, **"Act In Space"** hackathon organized by Space Agency of France and European Space Agency took place. One of the members of the jury of the hackathon was Deputy Director for Innovation of ISSP UL Dr.phys. Andris Anspoks. Two of hackathon's mentors were representatives from ISSP UL - Dr.phys. Ilze Aulika and Dr.phys. Sergejs Fomins.
- On November 13, on LTV1 program **Rīta Panorāma** (*Morning Panorama*) story about transparent antibacterial coatings for screens and their possible application in fight against SARS-CoV-2 was broadcasted. The research was carried out within the framework of NRP project "Mitigation of Covid-19 effects". Head of the ISSP UL's Laboratory of Thin Films Dr. Juris Purāns and leading researcher Dr. Mārtiņš Zubkins told about their progress in research.

https://ltv.lsm.lv/lv/raksts/13.11.2020-izstrada-antibakterialu-caurspidigu-parklajumu-ekraniem.id202098/

- On December 2, the scope of the **ISO certificate 9001:2015** was extended. Currently certificate includes open access laboratory maintenance service, handling of equipment, design and development of products and services, procurement management, provision of the cleanroom infrastructure services for research, study process and innovation development.
- On December 4, ISSP UL hosted one of **BETA practical seminars** for secondary school students to promote the development of individual competencies of students in general education institutions. 36 secondary school students participated from all around Latvia. The seminar was hosted by ISSP UL's Deputy Director for Education Dr.phys. Anatolijs Šarakovskis, and researchers from ISSP UL's Laboratory of Prototyping of Electronic and Photonic Devices Dr.sc.ing. Gatis Mozoļevskis and Dr.sc.ing. Roberts Rimša.
- On December 5, one of the guests of the Rīga TV24 program "**Dr. Apinis**" was ISSP UL's Deputy Director for Science Dr.habil.phys. Andris Šternbergs. The program was devoted to the newly elected LAS officials.

https://xtv.lv/rigatv24/video/8blGbj3BGn3-05_12_2020_dr_apinis_1_dala

https://xtv.lv/rigatv24/video/W3AGXbmYNJ5-05_12_2020_dr_apinis_2_dala

- On December 9, guest appearance in LR1 program "**Zināmais Nezināmajā**" (*Known in the Unknown*) by ISSP UL's researcher from Laboratory of Materials for Energy Harvesting and Storage Pēteris Lesničenoks, who told about conversion of wave energy into usable electricity.

https://lr1.lsm.lv/lv/raksts/zinamais-nezinamaja/zinatnieki-censas-vilnu-energiju-parverst-jau-lietojama-elektroe.a137614/

- On December 15, ISSP UL became a member of **Latvian IT cluster**.

- December 17, an article about receiver of Mikrotīkls scholarship, researcher of ISSP UL's Spectroscopy Laboratory Guna Krieķe and her promotion work "Erbium upconversion luminescence in transparent glass ceramics containing ternary fluoride nanocrystals" was published on University of Latvia Fund homepage.

https://www.fonds.lv/par-mums/zinas/zina/t/62552/

- December 20, an interview with the leading researcher of the ISSP UL's Spectroscopy Laboratory, Dr. Andris Antuzevičs was published in the homepage of the **National Encyclopedia (NE) of Latvia**. In it he tells how the entries of NE on physics terms are written and also about his work in the ISSP UL's Laboratory of Spectroscopy, as well as the work as a lecturer at the UL's FPMO.

https://enciklopedija.lv/tapsana/108283-Saprotami-par-fiziku

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