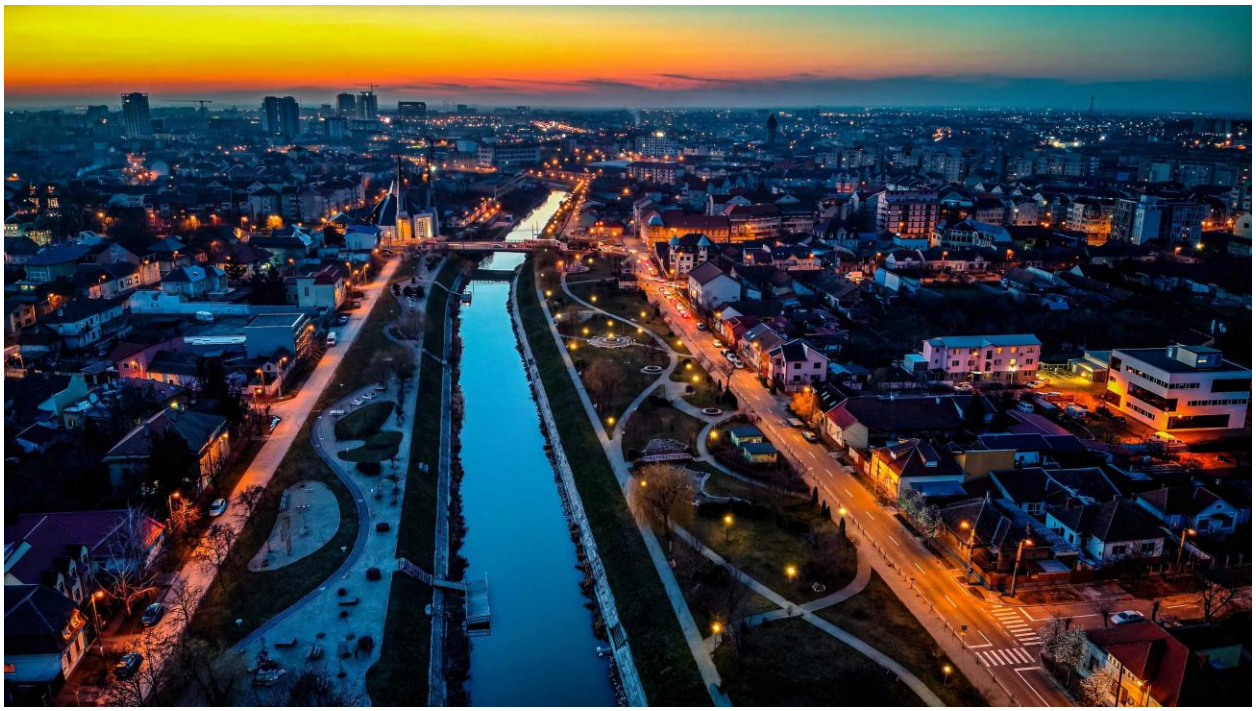

EuroDIM 15

The 15th Europhysical Conference on Defects in Insulating Materials

BOOK OF ABSTRACTS

July 06-10, 2026, Timisoara, Romania

Organized by:

Universitatea de Vest din Timişoara

FFM

SRF Societatea Română de Fizică Fondată 1890

Dear Colleagues,

It is our great pleasure to welcome you the 15th Europhysical Conference on Defects in Insulating Materials (EuroDIM-15), held at West University of Timisoara, Timisoara, Romania from July 06-10, 2026. Timisoara, also called "Little Vienna", is a strong university center and in 2023 it held the title of the cultural capital of Europe.

EuroDIM-15 continues the tradition of fourteen previous international conferences of bring together researchers from university, industry, and government laboratories around the world to report on the latest advances studies of defects in insulating materials.

EuroDIM-15 will provide a great opportunity to exchange ideas, allowing for fruitful discussions between industrial, academic, and scientific participants from various fields. The conference will include plenary, keynotes, invited, oral and poster sessions. EuroDIM-15 is the biggest event of this kind worldwide, occurring once every 4 years, and details of this edition may be found on the conference website https://eurodim.ro/.

We look forward to welcoming you to the Conference!

Warm regards,

EuroDIM-15 Chairs

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EuroDIM 2026
Timișoara, Romania, 2026

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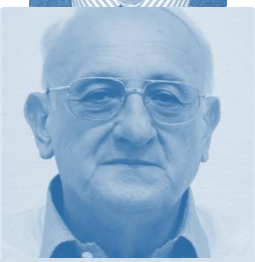
Roberto Lorenzi (Italy)

Siegmund Greulich-Weber (Germany)

Volkmar Dierolf (USA)

Yuriy Zorenko (Poland)

Plenary Speakers

1		**Anatoli Popov,** University of Latvia, Riga, Latvia	*Radiation defects in insulating materials: from early understanding to open challenges*
2		**Rob Jackson**, Keele University, UK	*Computer modelling of defects in insulating materials*
3		**Mikhail Brik**, University of Tartu, Tartu, Estonia	*First-principles and machine learning methods for description of substitutional defects in optical materials*
4		**Wieslaw Strenk**, Institute of Low Temperatures and Structure Research, Wroclaw Poland	*Modelling of laser-induced white emission of graphene*
5		**Tomoyuki Yamamoto**, Waseda University, Tokyo, Japan	*First principles calculations and machine learnings for the development of optical materials*

6		**Martin Albrecht**, Leibniz-Institut für Kristallzüchtung, Berlin, Germany	*Antisite defects in $SrTiO_3$: when off-stoichiometry turns disorder into function*
7		**Matias Velazquez**, CNRS-Grenoble INP-UGA, France	*Czochralski growth of large radiopure Li_2MoO_4 single crystals for heat- scintillation cryogenic bolometers*

* **Plenary lectures** are given in Plenary Sessions. They last 45 minutes + 5 minutes for discussion – **50 minutes in total.**

Keynote Speakers

1		**Daniel Vizman,** West University of Timisoara, Romania	*Controlled growth and characterization of Tb/Tm-doped fluoride single crystals*
2		**Maksym Buryi**, Institute of Plasma Physics, The Czech Academy of Sciences, Czech Republic	*Coupling cesium lead bromide perovskite with organic or inorganic compounds for improved stability and luminescence properties*
3		**Lengyel Krisztian**, HUN-REN Wigner Research Centre for Physics Institute for Solid State Physics and Optics, Budapest, Hungary	*Intrinsic and extrinsic defects in $LiNbO_3$ nanocrystals*
4		**Robert Tomala**, Institute of Low Temperature and Structure Research, Poland	*Luminescent nanoparticles for white light generation*
5		**Yuriy Zorenko**, Kazimierz Wielki University, Poland	*Luminescence of defects and isoelectronic impurities in UV-emitting oxide scintillators under X-ray and synchrotron radiation excitation*

6		**Virgīnija Vītola**, University of Latvia, Latvia	*Laser-patterned direct-write afterglow coatings for road safety*
7		**Marius Stef**, West University of Timisoara, Romania	*Growth and characterization of rare-earth doped fluorite luminescent crystals*
8		**Mario Valerio,** Federal University of Sergipe, Brazil	*Crystal field–driven luminescent thermometry in Nd^{3+}-doped yttrium oxyfluorides: linking structure and Stark level splitting*
9		**Florentina Neatu**, European Comission, Bruxelles, Belgium	*ERC Grants: From funding opportunities to proposal evaluation*
10		**Shunsuke Kurosawa,** Nagoya University	*Radiation hardness of scintillation materials with high effective atomic number*

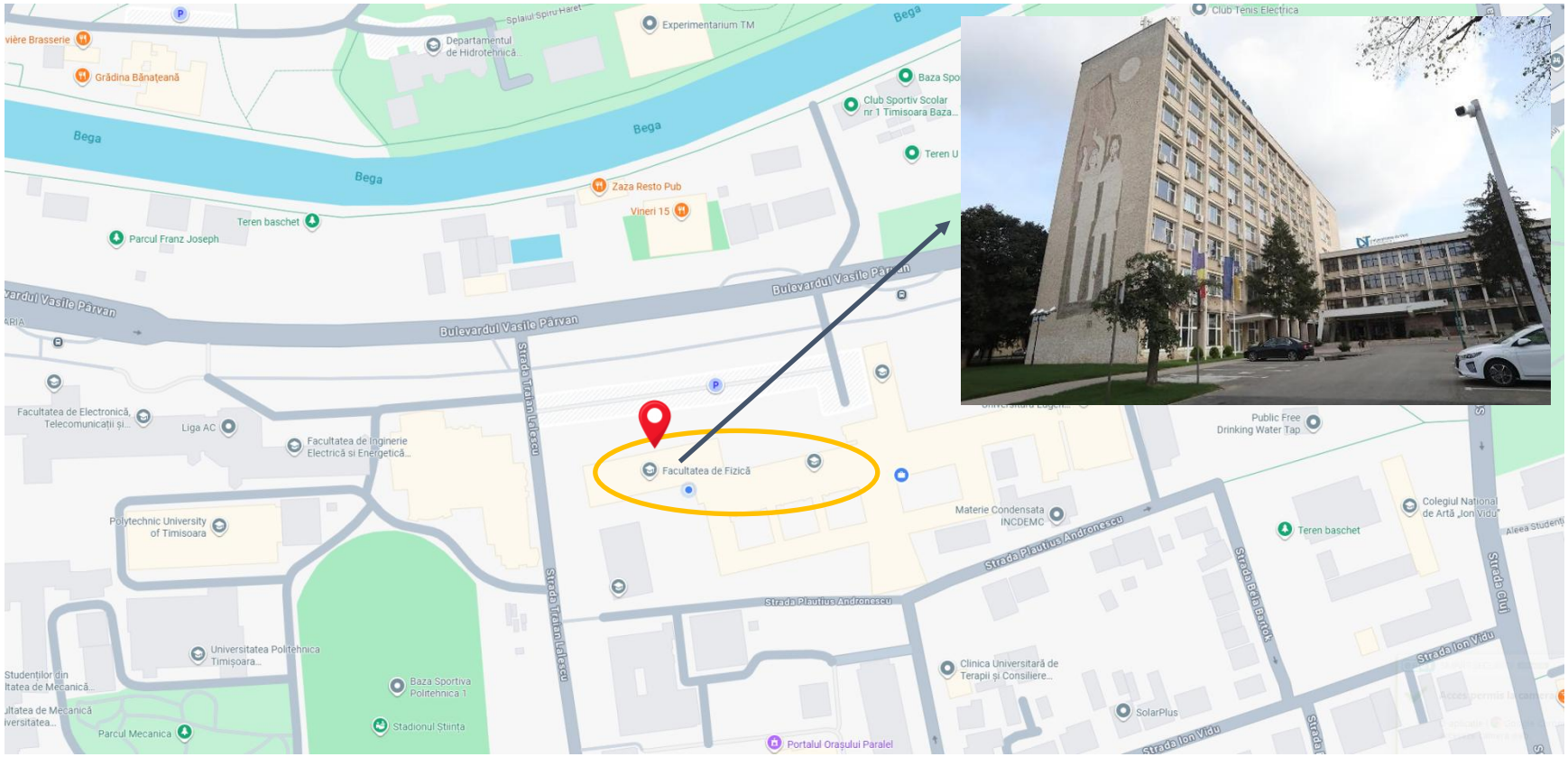
* **Keynote lectures:** 30 minutes + 5 minutes for discussion – **35 minutes in total**.

Invited Speakers

1	Aleksandr Lushchik, University of Tartu, Tartu, Estonia	*Characterization of oxygen-related Frenkel defects induced by energetic neutrons or ions in functional metal oxides*
2	Henk Vrielinck, Ghent University, Gent, Belgium	*Reading without erasing: A study of trapped charges in radiochromic and radio-photoluminescence phosphors*
3	Shelja Sharma, University of Latvia, Latvia	*Morphology-controlled Er-doped ZnO nanorods with enhanced NIR emission and defect modulation*
4	Inesh Kenzhina, Satbayev University, Almaty, Kazakhstan	*The role of structural defects caused by irradiation on the change in the properties of ceramic materials – promising materials for nuclear energy*
5	Irene Villa, University of Milano-Bicocca, Milano, Italy	*The Impact of structure and composition on fast-emitting lightweight hybrid scintillators*
6	Francesca Cova, University of Milano-Bicocca, Milano, Italy	*Role of localized electronic levels in scintillating materials for high-energy radiation detection*
7	Gheorghe Lucian, National Institute for Laser, Plasma and Radiation Physics, Magurele, Romania	*LGYSB:Nd crystal: Czochralski growth, optical properties, and NIR laser emission performances*
8	Silviu Polosan, National Institute of Materials Physics, Magurele, Romania	*Oxygen defects and ferroelectricity of $BaFe_{12}O_{19}$ hexaferrites*
9	Sergiu Vatavu, Moldova State University, Republic of Moldova	*Technology aspects of high-entropy oxides preparation by metalorganic aerosol deposition*
10	Simonpietro Agnello, University of Palermo, Italia	*2D MoS_2 from thermal stability to irradiation induced modifications*
11	Philippe Veber, West University of Timisoara, Romania	*SMART Growth: Artificial intelligence enhanced for sustainable growth of rare-earth materials based laser*
12	Mamoru Kitaura, Yamagata University, Yamagata, Japan	*Impact of impurity doping on vacancy type defects in functional materials revealed by positron annihilation spectroscopy*

Venue

West University of Timisoara, Bd. Vasile Parvan 4, Timisoara



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EuroDIM-15 Timetable

Sunday July 5th	Monday July 6th	Tuesday July 7th	Wednesday July 8th	Thursday July 9th	Friday, July 10th
ESDIM-1	8:30 – 14:00 Registration	8:30 – 14:00 Registration	**8:00, 8:30 – 19:00** Corvin Castle excursion (including **Lunch**)	9:30 – 11:30 PL-06, K-05, K06 (**Aula Magna**)	9:00 – 9:50 PL-09 (**Aula Magna**)
	09:30-10:00 Opening ceremony (**Aula Magna**)	09:00 – 11:30 PL-03, PL-04, PL-05 (**Aula Magna**)		11:30 – 12:00 Coffee break (1st floor)	09:50 – 10:10 Coffee break (1st floor)
	10:00 – 11:40 PL-01, PL-02 (**Aula Magna**)				10:00 – 11:20 K-09, K-10 (**Aula Magna**)
	11:40 – 12:00 Coffee break (1st floor)	11:30 – 12:00 Coffee break (1st floor)		12:00 – 13:10 K-07, K-08 (**Aula Magna**)	11:20 Closing ceremony (**Aula Magna**)
	12:00 – 13:10 K-01, K-02 (**Aula Magna**)	12:00 – 13:10 K-03, K-04 (**Aula Magna**)		13:15 – 15:00 Lunch (Vineri15)	Departure of participants
	13:15 – 14:50 Lunch (Vineri15)	13:15 – 14:50 Lunch (Vineri15)		15:00 – 16:30 **Room A01** I-11, O-11, O-12, O-13 **Room A11** I-12, O-14, O-15, O-16	
	15:00 – 16:40 **Room A01** I-01, I-02, O-01, O-02 **Room A11** I-03, I-04, O-03, O-04	15:00 – 16:10 **Room A01** I-09, O-07, O-08 **Room A11** I-10, O-09, O-10		18:00 – 22:00 Social dinner (Recas winery)	
	16:40 – 17:10 Coffee break (1st floor)	16:10 – 17:00 Coffee break (1st floor)			
16:00 – 20:00 Registration	17:10 – 19:00 **Room A01** I-05, I-06, O-05 **Room A11** I-07, I-08, O-06	17:00 – 19:00 Poster session in front of Aula Magna			
19:00 – 21:00 Welcome reception (Vineri15)	19:00 – 21:00 Dinner (Vineri15)	19:00 – 21:00 Dinner (Vineri15)	19:00 – 21:00 Dinner („Sura”, Dumbrava)		

- Plenary session 50 min. (including 5 min. discussions) → Aula Magna
- Keynote session 35 min. (including 5 min. discussions) → Aula Magna
- Invited session 30 min. (including 5 min. discussions) →A01, A11
- Oral session 20 min. (including 5 min. discussions) →A01, A11

EuroDIM-15 program

Sunday, 5th of July 2026	
16:00 – 20:00	Participants Registration Desk Open – in front of Aula Magna
19:00 – 21:00	**Welcome reception** (Restuarant "Vineri 15" - across from the university)

Monday, 6th of July 2026		
08:30 – 14:00		Participants Registration Desk Open – in front of Aula Magna
09:30 – 10:00		Opening Ceremony (Aula Magna)
Plenary Session 1 (Aula Magna) *Chairman: Daniel Vizman*		
10:00 – 10:50	**PL-01**	**Czochralski growth of large radiopure Li_2MoO_4 single crystals for heat-scintillation cryogenic bolometers** M. Velázquez*, C. Stelian, N. Kaoutar, I. Nuta, G. Deffrennes *Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMAP, 38000 Grenoble, France*
10:50 – 11:40	**PL-02**	**First-principles and machine learning methods for description of substitutional defects in optical materials** M.G. Brik[1,2,3,4*] [1]*Institute of Physics, University of Tartu, W. Ostwald Str. 1, Tartu, 50411, Estonia* [2] *Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Serbia* [3] *Faculty of Science and Technology, Jan Długosz University, Armii Krajowej 13/15, PL-42200, Częstochowa, Poland* [4] *School of Integrated Circuits, Chongqing University of Posts and Telecommunications, Chongqing, PR China*
11:40 – 12:00		Coffee Break – UVT Cafeteria 1st floor
Keynote Session 1 (Aula Magna) *Chairman: Matias Velazquez*		
12:00 – 12:35	**K-01**	**Crystal field–driven luminescent thermometry in Nd^{3+}-doped yttrium oxyfluorides: Linking structure and Stark level splitting** Renato Willy Vieira de Oliveira [1], Bárbara Matos Cruz [1], Tatiane S. Lilge [1,2], Adriano, B. Andrade [1], Ruan. P. R. Moura [3], José Joatan Rodrigues Jr. [3], Márcio A.R.C. Alencar [3], Robert A. Jackson [4], Mário E. G. Valerio [1*] and Zélia S. Macedo [1] [1]*Laboratory of Preparation and Characterization of Materials (LPCM), Department of Physics, Federal University of Sergipe, São Cristóvão−SE, Brazil* [2]*Graduate Program in Materials Science and Engineering, Laboratory of Glass-Ceramic Materials (VITROCER), Federal University of Santa Catarina, Florianópolis, SC, Brazil* [3]*Laboratory of Corrosion and Nanotechnology (LCNT), Federal University of Sergipe, São Cristóvão 49107-230, Brazil* [4]*School of Chemical and Physical Sciences, Keele University, Keele, Staffordshire, ST5 5BG, UK*
12:35 – 13:10	**K-02**	**Radiation hardness of scintillation materials with high effective atomic number** Shunsuke Kurosawa[1*], [1]*Nagoya University: Graduate School of Eng., Nagoya, Japan*
13:15 – 14:50		Lunch (Restaurant "Vineri 15" - across from the university)

	Oral sessions 1	
15:00 – 16:40	Room A01 *Chairman: Robert Tomala*	Room A11 *Chairman: Krisztian Lengyel*
15:00 – 15:30	*Invited* **I-01. Impact of impurity doping on vacancy type defects in functional materials revealed by positron annihilation spectroscopy** Mamoru Kitaura* *Faculty of Science, Yamagata University, Yamagata 990-8560, Japan*	*Invited* **I-03. LGYSB:Nd crystal: Czochralski growth, optical properties, and NIR laser emission performances** Gheorghe Lucian*, Broasca Alin, Greculeasa Madalin, Voicu Flavius, Hau Stefania, Gheorghe Cristina, and Croitoru Gabriela *National Institute for Laser, Plasma and Radiation Physics, 409 Atomistilor, 077125 Magurele, Romania*
15:30 – 16:00	*Invited* **I-02. Oxygen defects and ferroelectricity of $BaFe_{12}O_{19}$ hexaferrites** Silviu Polosan*, Corina Secu, Catalin Negrila, Andrei Nitescu and Mihai Secu *National Institute of Materials Physics, Magurele, Romania*	*Invited* **I-04. The role of structural defects caused by irradiation on the change in the properties of ceramic materials – promising materials for nuclear energy** Kenzhina I.E.[1,2*], Kozlovskiy A.L.[1,2], Zhigalova A.[3] *[1] Satbayev University, Almaty, Kazakhstan* *[2]Institute of Nuclear Physics of the ARKAE, Almaty, Kazakhstan* *[3]L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*
16:00 – 16:20	**O-01. Electronic and optical properties of YVO_4:Eu induced by different charge states of the Eu ion: an ab-initio study** F.O. Carvalho, O. M. Sousa, G.J. Piropo, A.F. Lima, M.V. Lalic *Physics Department, Federal University of Sergipe, 49100-000, São Cristóvão, Brazil*	**O-03. Development of Nd-doped LGSB crystals as new candidates for the next generation of bifunctional crystals** Madalin Greculeasa*, Alin Broasca, Flavius Voicu, Cristina Gheorghe, Stefania Hau, Catalina-Alice Susala, Nicolaie Pavel, Lucian Gheorghe *National Institute for Laser, Plasma and Radiation Physics, ECS Laboratory, P.O. Box MG- 36, 077125 Magurele, Romania*
16:20 – 16:40	**O-02. Swift heavy-ion induced defect formation and luminescence modification in Ce-doped garnet single crystalline films** Alma Dauletbekova[1], Vitalii Gorbenko[2], Abdirash Akilbekov[1], Nuraiym Pirzadayeva[1], Tetiana Zorenko[2], Gulnara Aralbayeva[1], Yuriy Zorenko[2,3] *[1]Department of Technical Physics, L.N. Gumilyov Eurasian National Universit? Astana, Kazakhstan* *[2]Physical Faculty of Kazimierz Wielki University in Bydgoszcz, Bydgoszcz, Poland* *[3]Medical Physics Department, F. Lukaszuk Oncology Center,Bydgoszcz, Poland*	**O-04. High-performance multi-wavelength laser emission from a newly developed Nd-doped LYSB crystal** Alin Broasca*, Madalin Greculeasa, Flavius Voicu, Cristina Gheorghe, Stefania Hau, Gabriela Croitoru, Lucian Gheorghe *National Institute for Laser, Plasma and Radiation Physics, 077125 Magurele, Romania, Solid-State Quantum Electronics Laboratory*
16:40 – 17:10	Coffee Break – UVT Cafeteria 1st floor	
	Oral session 2	

17:10 – 19:00	Room A01 *Chairman: Gheorghe Lucian*	Room A11 *Chairman: Silviu Polosan*
17:10-17:40	*Invited* **I-05. SMART Growth: Artificial intelligence enhanced for sustainable growth of rare-earth materials based laser** Philippe Veber[*1,2], Dragos Tatomirescu[1], Alexandra Popescu[1], Gabriel Buse[2], Daniel Vizman[1], Natasha Dropka[3] *[1]Faculty of Physics, Crystal growth laboratory, West University of Timisoara (Romania)* *[2]Institute for Advanced Environmental Research (ICAM), West University of Timisoara (Romania)* *[3]Leibniz Institute for Crystal Growth, IKZ, Berlin (Germany)*	*Invited* **I-07. Characterization of oxygen-related Frenkel defects induced by energetic neutrons or ions in functional metal oxides** Aleksandr Lushchik*, Aleksei Krasnikov, Viktor Seeman, and Evgeni Shablonin *Institute of Physics, University of Tartu, W. Ostwald Str. 1, 50411 Tartu, Estonia*
17:40-18:10	*Invited* **I-06. Technology aspects of high-entropy oxides preparation by metalorganic aerosol deposition** Alexandru Varzari[1], Gheorghe Ghiletchii[1], Oleg Shapoval[1], Alexandr Belenchuk[1], Marin Rusu[1], Petronela Garoi[2], Valentin Craciun[2], Ștefan-Andrei Irimiciuc[2,3] and Sergiu Vatavu[1*] *[1]Physics of Semiconductors and Devices Laboratory, Faculty of Physics and Engineering, Moldova State University, 60 A. Mateevici str., Chișinău, MD-2009, Moldova* *[2]National Institute for Laser, Plasma and Radiation Physics, Magurele 077125, Romania* *[3]Institute of Physics of Czech Academy of Sciences, Na Slovance 1999/2, 182 00 Prague, Czech Republic*	*Invited* **I-08. Reading without erasing: A study of trapped charges in radiochromic and radio-photoluminescence phosphors** Henk Vrielinck[1*], Zetian Yang[2], Emiel Botterman[1,2], Eliot Janssens[1,2], David Van der Heggen[2], Philippe F. Smet[2] and Dirk Poelman[2] *[1]Research group Defects in SemiConductors, Ghent University-Dept. Solid State Sciences, Krijgslaan 285-S1, B-9000 Gent, Belgium* *[2]LumiLab, Ghent University-Dept. Solid State Sciences, Krijgslaan 285-S1, B-9000 Gent, Belgium*
18:10-18:30	**O-05. Control of the emission wavelength of Cs_2HfCl_6 via tetravalent ion doping** Chihaya Fujiwara[1,2*], Akihiro Yamaji[3], Akira Yoshiakwa[1] and Shunsuke Kurosawa[3,4] *[1]Institute for Materials Research, Tohoku University, Sendai, Japan* *[2]Department of Materials Science, Graduate School of Engineering, Tohoku University, Sendai, Japan* *[3]Graduate School of Engineering, Nagoya University, Nagoya, Japan* *[4]Institute of Laser Engineering, Osaka University, Osaka, Japan*	**O-06. Multi-spectroscopic studies of defects in quartz as a natural dosimeter** Alida Timar-Gabor[1,2*] and PROGRESS team members *[1]Faculty of Environmental Science and Engineering, Babeş-Bolyai University* *[2]Institute for Interdisciplinary Research in Bio-Nano-Science, Babeş-Bolyai University, Cluj-Napoca, Romania*
19:00-21:00	Dinner – Restaurant “Vineri 15”	

Tuesday, 7th of July 2026		
08:30 – 14:00	Participants Registration Desk Open – in front of Aula Magna	
Plenary Session 2 (Aula Magna) *Chairman: Mikhail Brik*		
09:00 – 09:50	**PL-03**	**Computer Modelling of Defects in Insulating Materials** Robert A Jackson* *School of Chemical and Physical Sciences, Keele University, Keele, Staffordshire ST5 5BG,*
09:50 – 10:40	**PL-04**	**First principles calculations and machine learnings for the development of optical materials** Tomoyuki Yamamoto[1*, 2, 3] [1]*Faculty of Science and Engineering, Waseda University, Tokyo, Japan* [2]*Kagami Memorial Research Institute for Materials Science and Technology , Waseda University, Tokyo, Japan* [3]*Institute of Condensed Matter Science, Waseda University, Tokyo, Japan*
10:40 – 11:30	**PL-05**	**Modelling of laser-induced white emission of graphene** W. Strek, R. Tomala, P. Wiewiórski, M. Stefański *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland*
11:30 – 12:00	Coffee Break – UVT Cafeteria 1st floor	
Keynote Session 2 (Aula Magna) *Chairman: Robert Jackson*		
12:00 – 12:35	**K-03**	**Controlled growth and characterization of Tb/Tm-doped fluoride single crystals** Marius Stef[1], Carla Schornig[1], Gabriel Buse[2], Maria Poienar[2], Philippe Veber[1], and Daniel Vizman[1*] [1]*Faculty of Physics and Mathematics, West University of Timisoara, Timisoara, Romania* [2]*Institute for Advanced Environmental Research, West University of Timisoara, Timisoara, Romania*
12:35 – 13:10	**K-04**	**Coupling Cesium Lead Bromide Perovskite with Organic or Inorganic Compounds for Improved Stability and Luminescence Properties** Maksym Buryi[1]*, Tomáš Hostinský[1,2], Jan Zich[1,2] [1]*Institute of Plasma Physics of the Czech Academy of Sciences, U Slovanky 2525/1a, 182 00 Prague, Czechia* [2]*Faculty of Chemical Technology, University of Pardubice, Studentská 95, 532 10 Pardubice 2, Czech Republic*
13:15 – 14:50	Lunch (Restaurant "Vineri 15" - (across from the university)	
	Oral sessions 3	
	Room A01 *Chairman: Philippe Veber*	Room A11 *Chairperson: Alida Gabor*
15:00 – 15:30	*Invited* **I-09. Morphology-controlled Er-doped ZnO nanorods with enhanced NIR emission and defect modulation** Shelja Sharma[1*], Jafar Fathi[1,2,4], Zdeněk Remeš[3], Andriy Prokhorov[3], Sergii Chertopalov[3] Maksym Buryi[1]* [1]*Institute of Plasma Physics of the Czech*	*Invited* **I-10. Role of localized electronic levels in scintillating materials for high-energy radiation detection** Francesca Cova[1*] [1]*Department of Materials Science, University of Milano – Bicocca, Milano, Italy*

	Academy of Sciences, U Slovanky 2525/1a, 182 00, Prague, Czech Republic *[2]Faculty of Environmental Sciences, Czech University of Life Sciences Prague, Kamýcká 129, Suchdol 165 00, Prague, Czech Republic* *[3]Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 182 00 Prague 8, Czech Republic* *[4]University of Chemistry and Technology, Technická 5, 166 28 Prague 6, Czech Republic*	
15:30 – 15:50	**O-07. Mapping defect energy levels in Ce-doped $KMgF_3$ via synchrotron-based X-ray spectroscopy** Giordano F. C. Bispo [1,2], Adriano B. Andrade[2], Davi H. S. Pedroso [3], Eduily B. V. Freire[4], Robert A. Jackson [5], Zélia S. Macedo[2,3], Thiago J. A. Mori[1], Tulio C. R. Rocha[1], Mário E. G. Valerio[2,3*] *[1] Brazilian Synchrotron Light Source (LNLS), Brazilian Center for Research in Energy and Materials (CNPEM), Campinas-SP, Brazil.* *[2] Laboratory of Preparation and Characterization of Materials (LPCM), Department of Physics, Federal University of Sergipe, São Cristóvão−SE, Brazil.* *[3] Materials Science and Engineering Postgraduation Programme (P2CEM), Federal University of Sergipe, São Cristóvão−SE, Brazil.* *[4] Postgraduate Program in Physics, Campus Ministro Petrônio Portella, Federal University of Piaui, Teresina−PI, Brazil.* *[5] School of Chemical and Physical Sciences, Keele University, Keele, Staffordshire, ST5 5BG, UK*	**O-09. UV-VUV induced thermally stimulated luminescence in scintillating crystals using synchrotron radiation** Roberto Lorenzi[1,*], Pietro Moiraghi[1], Vittoria Vigorito[1], Alessandra Ronchi[1], Jan Hostaša[2], Francesco Picelli[2], Alberto Paleari[1] and Francesca Cova[1] *[1]Department of Materials Science, University of Milano-Bicocca, Milan, Italy* *[2]CNR ISSMC, Institute of Science, Technology and Sustainability for Ceramics, Faenza, Italy*
15:50 – 16:10	**O-08. Structural and optical properties of YAG:Ce single-crystalline film phosphors under high-pressure and low-temperature conditions: impact of homo- and quasi-homoepitaxial growth** Y. Syrotych[1*], M. Kamiński[2], N. Majewska[2], V. Gorbenko[1], A. Wierzbicka[3], Y. Zhydachevskyy[3], S. Mahlik[2], and Yu. Zorenko[1] *[1] Faculty of Physics, Kazimierz Wielki University in Bydgoszcz, Powstańców Wielkopolskich str., 2, 85090 Bydgoszcz, Poland* *[2] Institute of Experimental Physics, Faculty of Mathematics, Physics and Informatics, University of Gdansk, Wita Stwosza 57, 80-308 Gdansk, Poland* *[3] Institute of Physics, Polish Academy of Sciences, al. Lotnikow 32/46, 02-668 Warsaw, Poland*	**O-10. Stability and synthesis attempt of novel A_2(Ce/Pr)WO_6 double perovskites (A=Ba, Sr, Ca) in the prospect of future energy conversion applications.** Damian Wlodarczyk[1*], Mikolaj Amilusik[2], Marcin Zajac[3], Lev-Ivan Bulyk[1], Sara Piotrowska[1], Roman Minikayev[1], Andrzej Suchocki[1†] *[1]Institute of Physics PAS, Ave. Lotnikow 32/46, PL-02-668, Warsaw, Poland* *[2]Institute of High Pressure PAS, Sokołowska 29/37, PL-01142, Warsaw, Poland* *[3]Solaris Synchrotron NSRC, Czerwone Maki 98, PL-30392, Krakow, Poland*

17:00 – 19:00	Poster session with refreshments (in front of Aula Magna) – *Chairman Marius Stef*
19:00 – 22:00	Dinner – Restaurant "Vineri 15"

Wednesday, 8th of July 2026	
08:00 – 20:00	**DAY TRIP: HUNEDOARA – CORVIN CASTLE + Lunch** **Confernce Photo** **Departure:** 08h00 AM and 08h30 AM (in front of the university) **Transport:** Modern air-conditioned coach, **Guide:** Licensed English-speaking tour guide
20:00 – 22:00	Dinner **"Șura"** restaurant, Dumbrava

Thursday, 9th of July 2026		
Plenary Session 3 (Aula Magna) *Chairman: Henk Vrielinck*		
09:30 – 10:20	**PL-06**	**Radiation defects in insulating materials: From early understanding to open challenges** Anatoli I. Popov *Institute of Solid State Physics, University of Latvia, Riga, Latvia*
Keynote Session 2 (Aula Magna) *Chairman: Henk Vrielinck*		
10:20 – 10:55	**K-05**	**Luminescent nanoparticles for white light generation** R. Tomala*, M. Chaika, A. Musialek, W. Strek [1]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland*
10:55 – 11:30	**K-06**	**Laser-patterned direct-write afterglow coatings for road safety** Virgīnija Vītola[1*], Katrīna Križmane[1] and Krišjānis Šmits[2] [1]*Author affiliation: Institute of Solid State Physics, University of Latvia, Riga, Latvia* [2]*Author affiliation: SIA "R4ST", Riga, Latvia*
11:30 – 12:00	Coffee Break – UVT Cafeteria 1st floor	
Keynote Session 3 (Aula Magna) *Chairman: Virgīnija Vītola*		
12:00 – 12:35	**K-07**	**Growth and characterization of rare-earth doped fluorite luminescent crystals** Marius Stef[1*], Carla Schornig[1], Philippe Veber[1], Gabriel Buse[2], Maria Poienar[2], Irinuca Bodea[1] and Daniel Vizman[1] [1]*Faculty of Physics and Mathematics, West University of Timisoara, Timisoara, Romania* [2]*Institute for Advanced Environmental Research, West University of Timisoara, Timisoara, Romania*
12:35 – 13:10	**K-08**	**ERC grants: From funding opportunities to proposal evaluation** Florentina Neatu *Executive Agency (ERCEA), European Commission*
13:15 – 14:50	Lunch (Restaurant "Vineri 15" - (across from the university)	
	Oral session 4, room A01 *Chairperson: Inesh Kenzhina*	Oral session 5, room A11 *Chairperson: Alin Broască*

15:00 – 15:30	*Invited* **I-11. The impact of structure and composition on fast-emitting lightweight hybrid scintillators** Irene Villa[1] [1]*Department of materials Science, University of Milano-Bicocca, Milan, Italy*	*Invited* **I-12. 2D MoS_2 from thermal stability to irradiation induced modifications** S. Agnello[1,2*], A. Madonia[1], E. Sangiorgi[1], F. Migliore[1], M. Cannas[1], G. Buscarino[1], A. Alessi[3], S.E. Panasci[4], E. Schiliro'[4], F. Giannazzo[4], L. Seravalli[5] [1]Author affiliation: D*epartment of Physics and Chemistry Emilio Segre', University of Palermo, Palermo, Italy* [2]Author affiliation: *AtenCenter, University of Palermo, Palermo, Italy* [3]Author affiliation: *LSI, CEA/DRF/IRAMIS, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, France* [4]Author affiliation: *Consiglio Nazionale delle Ricerche - IMM, Catania, Italy* [5]Author affiliation: *Consiglio Nazionale delle Ricerche - IMEM, Parma, Italy*
15:30 – 15:50	**O-11. Luminescence dynamics of $CsPbI_3$ perovskite nanocrystal scintillators** V. Vigorito[1*], F. Cova[1], R. Lorenzi[1], A. Paleari[1], V. Bellotti[1], A. Ronchi[1], F. Locardi[2], D. Pratolongo[2], S. Nargelas[3], G. Soltanaitė[3], I. Veronese[4], and M. Fasoli[1] [1]*Department of Materials Science, University of Milano-Bicocca, Milan, Italy* [2]*Department of Chemistry and Industrial Chemistry, University of Genova, Genoa, Italy* [3]*Department of Physics, Vilnius University, Vilnius, Lithuania* [4]*Department of Physics, University of Milano, Milan, Italy*	**O-14. Comparison of optical properties of Ga-doped ZnO thin films and NV rich single crystal diamond** Zdenek Remes[1], Josef Soucek[1,2], Neda Neykova[1,3] [1]*FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague, Czechia* [2]*Czech Technical University in Prague, Faculty of Biomedical Engineering, nám. Sítná 3105, 272 01 Kladno, Czechia* [3]*Faculty for Electrical Engineering,Czech Technical University in Prague, Technická 2, 166 27 Prague,Czech Republic*
15:50 – 16:10	**O-12. Diopside photocatalyst from agro-industry waste: Revolutionizing sustainable** wastewater treatment Gangadhar Mahar[1,2,3], Sushil Patel[1,2], Pooja Yadav[1,2], Michal Piasecki[3], P Abdul Azeem[1,2]* [1]*Department of physics, National Institute of Technology, Warangal, India, 506004* [2]*Centre for Glass Science and Technology, National Institute of Technology, Warangal, India, 506004* [3]*Department of physics, Jan Dlugosz University in Czestochowa, Poland*	**O-15. Structural and thermodynamic stabilization of $Li_{1.2}Mn_{0.8}O_2$ cathodes through Ti doping: Insights from DFT and cluster expansion** M.E. Kgoedi [1*], N.N. Ngoepe[1], M.C. Masedi[1], R.S. Ledwana[1] and P.E. Ngoepe[1] [1]*Materials Modelling Centre, University of Limpopo, Private Bag x1106, Sovenga 0727, South Africa.*
16:10 – 16:30	**O-13. Delithiation and temperature-induced behaviour in a Li_2MnO_3-$Li_{0.69}MnO_2$ core-shell system: A molecular dynamics study** P.G. Makhubela[1*], P.E. Ngoepe[1], K.M. Kgatwane[1] and R.S. Ledwaba[1] [1] *University of Limpopo, Materials Modelling*	**O-16. Interplay of optically- and magnetoactive energy levels of the Ce-doped $Y_3Al_5O_{12}$ nanopowders** K. Lamonova[1*], Yu. Kazarinov[2], I. Danilenko[1,3], and O. Gorban[1.3] [1]*O. O. Galkin Donetsk Institute for Physics and Engineering, NAS of Ukraine, Kyiv, Ukraine*

	Centre, Polokwane, South Africa.	[2]*NSC Kharkiv Institute of Physics and Technology, NAS of Ukraine, Kharkiv, Ukraine* [3]*Nanomatetials Research&Development, Krakow, Poland*
16:30 – 17:30	**Meeting of International Advisory Committee (Room A01)**	
18:00 – 22:00	**Social dinner (Recas winery)** **Departure:** 18h00 and 18h30 (in front of the university) **Transport:** Modern air-conditioned coach **Anouncement of the poster prizes** Committee *Maksym Buryi* *Robert Jackson* *Mikhail Brik* *Marius Stef*	

Friday, 10th of July 2026		
Plenary Session 4 (Aula Magna) *Chairman: Maksym Buryi*		
09:00 –09:50	**PL-09**	**Antisite defects in $SrTiO_3$: when off-stoichiometry turns disorder into function** Martin Albrecht[1]*, Chang-Ming Liu[1], Wahib Aggoune[2], Alexander Meledin[3], Mohamed Abdeldayem[1], Thilo Remmele[1], Andreas Fiedler[1], Jutta Schwarzkopf[1], Matthias Scheffler[3], and Dan Zhou[1] [1] *Leibniz-Institut für Kristallzüchtung, Berlin, Germany* [2] *Fritz-Haber-Institute of the Max Planck Society, Berlin, Germany* [3] *Thermo Fisher Scientific Inc, Eindhoven, Netherlands*
09:50 – 10:10	Coffee Break – UVT Cafeteria 1st floor	
Keynote Session 4 (Aula Magna) *Chairman: Maksym Buryi*		
10:10 – 10:45	**K-09**	**Luminescence of defects and isoelectronic impurities in UV-emitting oxide scintillators under X-ray and synchrotron radiation excitation** Y. Zorenko[1,2,3], V. Gorbenko[1], S. Witkiewicz-Łukaszek[1], A. Majewski-Napierkowski[1], T. Zorenko[1], K. Shunkeyev[3], Sh. Sagimbayeva[3], A. Kenzhebayeva[3] [1]*Department of Physics of Kazimierz Wielki University,85-090 Bydgoszcz, Poland* [2]*Medical Physics Department, F. Lukaszuk Oncology Center, 85-796 Bydgoszcz, Poland* [3]*K. Zhubanov Aktobe Regional University, 030000 Aktobe, Kazakhstan*
10:45 – 11:20	**K-10**	**Intrinsic and extrinsic defects in $LiNbO_3$ nanocrystals** K. Lengyel[1*], L. Kocsor[1], G. Dravecz[1], L. Péter[1] [1]*Institute for Solid State Physics and Optics, HUN-REN Wigner Research Centre for Physics, Budapest, Hungary*
11:20	**Closing ceremony (Aula Magna)**	

Plenary session -abstracts-

PL-01. Czochralski growth of large radiopure Li_2MoO_4 single crystals for heat-scintillation cryogenic bolometers

M. Velázquez[1]*, C. Stelian[1], N. Kaoutar[1], I. Nuta[1], G. Deffrennes[1]
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Crucial experiments to discover the origin of the neutrino mass and the exact nature of neutrino particles require the detection of extremely rare events, such as the neutrinoless double beta decay ($2\beta0\nu$). The core of the most powerful detector that is being developed to detect $2\beta0\nu$ decays will be made of radiopure and 45 mm-edge cubic Li_2MoO_4 (LMO) single crystals assembled into vertical stacks (Fig. 1). Several massive LMO crystals (> 1 kg) were pulled, with a diameter 65 mm (Fig. 1). Three-dimensional (3D) modeling was applied to investigate heat transfer, convection and thermal stresses in Cz growth of LMO crystals. Several crystals of different diameters were grown in two different Cz configurations. The largest ingot grown in a furnace based on coupling the inductive coil and a platinum crucible (Cz1), has cracked as the bottom part of the crystal was cut. Another crystal, with larger diameter and length, was grown in a furnace based on inductive heating of a susceptor (Cz2), which was previously optimized by numerical modeling in order to reduce the thermal stresses in LMO crystals [1]. The thermal stress computations, carried out for the bulk LMO crystal grown in Cz1 configuration, show that the normal stress in the longitudinal section has a maximum which highly exceeds the critical value of the tensile stress in a region located at the bottom part of the ingot. That explains the fracture observed during the cutting of the ingot's tail. The computations performed in the Cz2 configuration case, dealing with LMO grown in an optimized setup, show that the crystal exhibits low thermal stress, except for a thin region of 2 mm located at the ingot periphery, where the stress slightly exceeds the critical value. We also show that thermal stresses can be reduced by a factor of 2 by growing the ingots parallel to the c-axis.

Simultaneously, we started modeling the K impurity solution thermodynamics of the Li- K-Mo-O system, since K, Th, U are the most undesirable radio-impurities in the crystal. Using the CALPHAD approach, we developed a thermodynamic database of the Li-Mo-O-K system in order to establish the physicochemical and thermodynamic conditions required for perfect control of synthesis and crystal growth conditions. We have obtained promising preliminary results, proving the robust solid-liquid and liquid-gas ternary congruence nature of LMO in equilibrium. Thanks to this phase diagram optimization and analysis including gas phases, we aim at modeling the equilibrium partition coefficient with the goal of designing a strategy to recycle very expensive ^{100}Mo-enriched remaining growth loads and LMO crystals scraps.

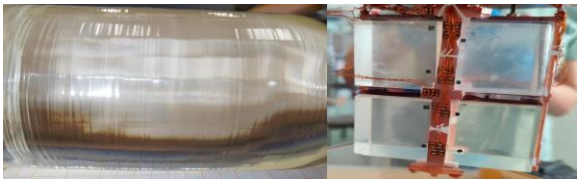

Figure 1: On the left, an Li_2MoO_4 single crystal, ≈1015 g and 65 mm in diameter; on the right, bolometers based on 45-mm edge cubic LMO crystals (≈280 g) cut from the as-grown boules (courtesy of Andrea Giuliani, IJCLab-Orsay).

References:

[1] C. Stelian, M. Velázquez "*3D numerical investigation of the factors affecting the thermal stresses and the wavy external shape of Li2MoO4 crystals grown by the Czochralski method*", J. Cryst. Growth, 658 (2025) 128134.

PL-02. First-principles and machine learning methods for description of substitutional defects in optical materials

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All applications of optical materials (scintillating, lighting, lasing, *etc*) stem from a complicated interplay of properties of crystalline hosts and artificially created defects, whose energy levels are located within the host's band gap. Among various kinds of defects in crystals, the substitutional defects (when one cation of a host matrix is replaced by another cation, usually from the transition metal or rare earth ions groups with unfilled 3d and 4f electron shells, respectively) play a special role. In this case, the optical transitions between the defects' energy levels located within the band gap of a host are utilized. Understanding the electronic properties of such systems is extremely important for their efficient application and improved performance.

In the present paper, the main attention is focused on crystalline matrices doped with Mn^{4+}, Ce^{3+}, Pr^{3+} ions used for lighting and scintillating applications. Examples of the Density Functional Theory (DFT) based calculations are described in detail to unveil the changes in the electronic properties of hosts after doping and to locate the impurity's ground state and its excited states with respect to the host's band structure [1-3]. Such calculations are important to understand and explain the existence or absence of impurity ions' emission in various hosts, the thermal stability of emission and the sensing properties of these materials. Additionally, examples of recently emerged machine learning methods in their application to the prediction of the emission properties of the above-mentioned impurity ions in crystals are also shown [4-5].

Keywords: DFT calculations, transition metal ions, rare earth ions, optical materials.

References:

[1] A.M. Srivastava, M.G. Brik, *J. Lumin.* **132**, 579-584 (2012).
[2] M.G. Brik, C.-G. Ma, M. Piasecki, A. Suchocki, *Opt. Mater.* **113**, 110843 (2021).
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[5] G. Dima, A.V. Racu, C.G. Ma, A.M. Srivastava, Ž. Antić, M.D. Dramićanin, M.G. Brik, *J. Lumin.* **286**, 121359 (2025).

PL-03. Computer modelling of defects in insulating materials

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Computer modelling of defects in insulating materials is a mature field, and for many years it has been a regular topic at the EURODIM/ICDIM conferences. This plenary lecture will provide an overview of work carried out by the author and collaborators, including results not presented previously at a -DIM conference, and will look ahead to the future and the latest developments in the field. I will also take some time to look at the history of the conference series (which is 70 years old this year, having started with a conference at Argonne in 1956 which focused on colour centres in alkali halides).

Materials to be discussed include UO_2 and other nuclear materials, $LiNbO_3$, and a range of mixed metal fluorides and oxides (noting that $LiNbO_3$ features regularly in this conference series).

Most calculations reported were performed using interatomic potentials, but comparison with DFT results is given where they are available, as well as the extent to which the results are comparable. Interatomic potentials were obtained using empirical fitting, but now machine learning (ML) based potentials are increasingly used, and their strengths and weaknesses will be discussed.

Keywords: Computer Modelling, Interatomic Potentials, Defects, Insulating Materials.

PL-04. First principles calculations and machine learnings for the development of optical materials

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It is essential to know the geometrical and electronic structures to understand the properties of the optical materials. Many of the current phosphor materials are realized by doping of rare-earth or 3d transition elements in the host materials with wide electronic band gap. In such cases, local environment of the doped ion is especially important to understand the luminescence property. To investigate such properties, first principles calculation is very powerful. Here the applications of the first principles calculations for the investigation of luminescence behaviour of the rare-earth free red phosphors, such as Mn^{4+} doped $CaAl_{12}O_{19}$ [1, 2] and Ca(Ti, Sn)O_3 [3], will be demonstrated.

In addition to the first principles calculations, a new type of technique using information technologies such as a machine learning technique, that is so called Materials Informatics (MI), has been widely used to develop new materials in these years. In the current work, applications of machine learnings to the predictions of 1) crystal structures of host materials of phosphors and 2) electronic properties, such as emission wave length and 10 Dq, will be displayed.

Keywords: first principles calculations, machine learning, rare-earth free red phosphor

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PL-05. Modelling of laser-induced white emission of graphene

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Laser induced broadband white emission was observed in several inorganic compounds and is preceded by multiphoton-induced ionization, giving access to broadband visible light. It is characterized by an excitation threshold, an exponential increase of emission intensity with excitation power, a saturation plateau, and an ejection of hot electrons giving access to efficient photocurrent. In present work we propose an empiric model of laser induced broadband emission and discuss its practical applications in lighting, photocurrent and photocatalysis.

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PL-06. Radiation defects in insulating materials: From early understanding to open challenges

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Since the early EURODIM meetings, including the conference held in Lyon in 1994, the field of radiation-induced defects in insulating materials has undergone remarkable development. Over the past decades, advances in experimental techniques, theoretical modeling, and computational approaches have significantly deepened our understanding of defect formation, structure, and dynamics under irradiation.

In this plenary lecture, I will present a retrospective overview of progress achieved since the 1990s in the study of radiation defects. I will highlight key milestones, including the identification and characterization of primary radiation-induced defects, the mechanisms of their creation and aggregation, and the development of microscopic models linking irradiation conditions to defect populations and their evolution. Particular emphasis will be placed on the relationship between radiation damage processes and the resulting changes in material properties.

Despite substantial progress, important challenges remain. I will discuss unresolved problems related to the complexity of radiation defect interactions, their evolution under high-energy irradiation, and non-equilibrium effects governing defect production and annealing. Limitations of current experimental resolution and predictive theoretical models will also be addressed, particularly in the context of multiscale radiation damage processes.

Finally, I will outline perspectives for future research, including the role of advanced spectroscopic techniques, first-principles simulations, and data-driven approaches in improving our understanding of radiation defect dynamics. A deeper control of radiation-induced defects remains crucial for the reliable design and performance of insulating materials in extreme radiation environments.

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PL-07. Antisite defects in $SrTiO_3$: when off-stoichiometry turns disorder into function

Martin Albrecht[1]*, Chang-Ming Liu[1], Wahib Aggoune[2], Alexander Meledin[3], Mohamed Abdeldayem[1], Thilo Remmele[1], Andreas Fiedler[1], Jutta Schwarzkopf[1], Matthias Scheffler[3], and Dan Zhou[1]

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The deliberate introduction of impurities to control electrical functionality is one of the foundational principles of semiconductor technology. In conventional semiconductors, substitutional doping tunes carrier concentration within a passive host lattice. In complex oxides, an analogous but richer design space opens through cation off-stoichiometry: point defects and their complexes introduce local polarity, switchable dipole configurations, and deep electronic states that can be engineered at the growth stage. This talk develops this idea through a concrete materials system, off-stoichiometric $SrTiO_3$, spanning atomic-scale defect physics, memristive device functionality, and, as a forward-looking perspective, physical reservoir computing.

Sr-deficient MOVPE growth produces Ti-on-Sr antisite defects coupled to Sr vacancies. These Ti_{Sr}–V_{Sr} complexes are deep, polar defects whose collective behaviour determines the observable device response. Atomic-resolution electron microscopy and first-principles theory converge on a consistent physical picture. In the bulk, electrostatic interactions drive the complexes toward mutually compensating dipole arrangements, suppressing macroscopic polarisation while establishing a landscape of metastable, history-dependent configurations; carrier transport proceeds through this landscape by hopping between neighbouring complexes via their localised deep gap states. At the interface, electric-field-driven reorientation of defect dipoles modulates the Schottky barrier and thereby controls carrier injection, providing the microscopic origin of both the resistance state and the observed switching asymmetry. The resulting device characteristics, forming-free, area-scaling, thickness-robust bipolar switching, are governed entirely by controllable point-defect chemistry, a direct oxide analogue of precision doping whose polar and many-body character produces functionality well beyond simple carrier modulation.

The same defect-ensemble offers a compelling extension toward physical reservoir computing. The hierarchy of dipole switching barriers, from fast, low-barrier reorientations to slow, voltage-driven collective rearrangements, gives rise to a multi-timescale dynamical spectrum whose dimensionality scales with the number of interacting complexes and is tunable through stoichiometry at the growth stage. These properties, high dimensionality, intrinsic recurrence, and synthesis-level designability, satisfy the central requirements of a physical reservoir computing substrate, and suggest cation off-stoichiometry in complex oxides as a route toward materials in which the capacity to process temporal information is an intrinsic, engineerable property of the crystal.

Keynote session -abstracts-

K-01. Luminescent nanoparticles for white light generation

R. Tomala*, M. Chaika, A. Musialek, W. Strek
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Recent advances in the design and optimization of luminescent nanoparticles for white light generation have been presented, with particular emphasis on rare-earth-doped oxide systems. It has been demonstrated that the crystalline environment strongly determines the spectroscopic properties of activator ions such as Ce^{3+} and Nd^{3+}, thereby enabling effective control of emission across the visible spectrum.

Strategies to improve the color rendering index (CRI) of phosphors for LED applications have been investigated. Bandgap engineering was achieved by modifying the host matrix composition, particularly by tuning the Al/Ga ratio in garnet structures. Co-doping with Cr^{3+} ions was applied to extend emission toward the red region of the spectrum, while nanocomposites incorporating carbon dots were developed to enhance excitation absorption and energy transfer efficiency [1]. It has been shown that combining these approaches enables precise tuning of emission intensity and spectral distribution.

Up-conversion processes in Nd^{3+}-doped oxide hosts have also been analyzed. Visible emission resulting from multiphoton excitation under near-infrared radiation has been observed. The coexistence of sharp f–f transitions and broadband phonon-assisted emission has been identified. Furthermore, the influence of temperature and pressure on up-conversion efficiency and spectral characteristics has been determined, indicating the possibility of controlling luminescent properties via external parameters.

The obtained results demonstrate that integrating down-conversion and up-conversion mechanisms into engineered nanomaterials is a promising approach for developing efficient white-light sources with tunable optical properties. Additionally, these systems exhibit potential for optical sensing, given their sensitivity of emission to environmental conditions.

The authors would like to acknowledge National Science Centre for financial support (Grant No. OPUS 23 UMO-2022/45/B/ST5/01487).

Keywords: white light, nanocrystals, lanthanides

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K-02. Intrinsic and extrinsic defects in $LiNbO_3$ nanocrystals

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Intrinsic and extrinsic defects in $LiNbO_3$ (LN) bulk crystals have been investigated with experimental and theoretical methods since many years. According to the most accepted model for the intrinsic defects in LN bulk crystals antisite niobium (Nb_{Li}) and lithium vacancy (V_{Li}) defects are present in the lattice in concentrations depending on the composition of the crystal. It was found by spectroscopic measurements that Er^{3+} and Yb^{3+} ions are incorporated on Li sites at low concentrations. Nowadays, the scientific attention has turned to nanocrystals (e.g., for quantum optic applications). One of the methods to reach nano-sized LN crystals is the frequently used ball-milling procedure. In this method, however, beside the reduction of the particle size to about 12-15 nm, the LN crystal structure is strongly altered, e.g., Li_2O leaves the lattice and a lithium-deficient phase, $LiNb_3O_8$ is formed [1]. Parallel to this structural change, the migration of rare-earth (RE) ions in the crystal lattice during milling is an important question for future applications. The feasibility of atomistic computer simulations (GULP) on ceria nanoparticles has been demonstrated. In addition, classical potential parameters for LN crystal were successfully developed, so a theoretical investigation of nano-sized undoped and rare-earth doped LN crystals became possible.

In the present work the results of spectroscopic measurements and theoretical calculations on undoped [1,2], Yb^{3+} and Er^{3+} doped LN nanocrystals [3] will be presented. The congruent LN crystals were grown by Czochralski method and ground under wet conditions in a high-energy ball mill in order to produce nanocrystals. The effect of size reduction to the crystal structure was monitored by Raman spectroscopy. The change of the environment of the RE^{3+} ions was followed by absorption measurement of the characteristic electronic transitions. For theoretical calculations a $Li_{245}Nb_{245}O_{735}$ unit, constructed from a 5x5x5 supercell by cutting off the sharp corners, was chosen as starting configuration with a size of about 24x24x52 $Å^3$. The relaxation of the unit was achieved by using conjugate gradient and subsequently Newton-Raphson optimization methods. The relaxation process was repeated with nano-LN structures containing Nb_{Li}+4V_{Li}, $LiNb_3O_8$ and RE^{3+}+2V_{Li} defect clusters. The total energies were compared in terms of both the defect positions and their relative locations.

Keywords: $LiNbO_3$, nanocrystal, rare earth ions.

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K-03. Controlled growth and characterization of Tb/Tm-doped fluoride single crystals

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Rare-earth-doped materials are key enabling materials for a wide range of photonic applications, including solid-state lasers, wavelength converters, magneto-optical components, scintillators and luminescent phosphors. In particular, fluorite-type hosts such as CaF_2 and BaF_2 have attracted sustained interest for visible and near-infrared photonics, due to their low multiphonon relaxation rates and high optical quality, which enable efficient emission and amplification processes, or magneto-optical properties. Tm^{3+} is a very interesting doping cation because of its electronic configuration, which allows several optical emissions at 1.5µm, 1.9µm and 2.3µm. Hence, Tm^{3+}-doped fluoride single crystals are promising for the realization of eye-safe laser, remote sensing of atmospheric species such as CH4, infrared counter-measurements or for medicine purposes. Tb^{3+}-doped single crystals are attractive materials for green photonic applications due to their low phonon energy, high optical transparency, and efficient Tb^{3+} emission. CaF_2 and BaF_2 single crystals doped with different TbF_3 concentrations (1, 5, and 10 mol%) and different TmF_3 content (0.1, 1 and 5 mol%) were grown by Bridgman technique [1-3] and systematically investigated in order to clarify the concentration-dependent spectroscopic behaviour of rare earth ions in a fluorite host. We focused on the influence of dopant concentration on optical absorption and UV-VIS luminescence behavior. Effective partitions coefficients of rare earth dopant in CaF_2 and BaF_2, which are of high importance for adjusting initial dopant content in the growth load in order to obtain as much as possible the final content of dopant in as-grown crystal, were calculated by two methods: ICP-MS coupled with LIBS and by optical absorption spectroscopy. Chemical characterization has shown that single crystals exhibit a highly homogenous [Tm] content distribution throughout the whole boule volume, but optical absorption measurements have displayed the presence of both Tm^{3+} and Tm^{2+} cations. The simultaneous presence of these cations is assumed to be likely due to the carbon environment and synproportionation partial reaction of TmF_3 which leads to Tm-mixed-valency-doped CaF_2 single crystals since Tm^{2+} can enter easily in the CaF_2 matrix because no charge compensation is needed. The results provide a consistent and detailed picture of the radiative behaviour of Tb and Tm ions in a fluorite-type host in the visible spectral range and clarify the role of concentration-dependent effects on their optical performance.

Keywords: fluoride crystals, crystal growth, rare-earth ions

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K-04. Coupling Cesium Lead Bromide Perovskite with Organic or Inorganic Compounds for Improved Stability and Luminescence Properties

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The incorporation of inorganic components such as MgO and ZnO leads to significant improvement in environmental stability and photoluminescence efficiency due to surface passivation, suppression of non-radiative recombination, and controlled charge transfer pathways. In particular, Mg incorporation into the perovskite lattice and interfaces reduces defect densities and prolongs luminescence decay times [1], while oxide-perovskite composites exhibit dual-phase excitonic emission and enhanced long-term stability. Embedding $CsPbBr_3$ nanocrystals into glass-ceramic or polymer matrices, including Eu-doped borophosphate glass-ceramics, further stabilizes the material and modifies charge trapping and recombination dynamics [2-4].

In addition to inorganic hosts, coupling with organic compounds, including diketopyrrolopyrrole (DPP)-based systems, was explored as a route to enhance light-harvesting and interfacial energy transfer. These organic-inorganic hybrid systems provide additional degrees of freedom for tailoring excitonic processes and improving stability under ambient conditions.

The results demonstrate that synergistic coupling of $CsPbBr_3$ with both inorganic oxides and organic functional molecules enables precise control over defect landscapes, excitonic recombination, and environmental robustness. This approach opens new pathways for the design of advanced perovskite-based materials for optoelectronic and scintillation applications.

Acknowledgements. The financial support of the Czech Science Foundation project No. 24-12872S and the program “Strategy AV 21” of the Czech Academy of Sciences, specifically work package VP 27 Sustainable Energy (Renewable energy resources and distributed energy systems) are gratefully acknowledged.

Keywords: Perovskite, ZnO, Polystyrene

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K-05. Crystal field–driven luminescent thermometry in Nd^{3+}-doped yttrium oxyfluorides: Linking structure and Stark level splitting

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Understanding the relationship between crystal structure and thermometric response remains a key challenge in luminescent thermometry, particularly in systems with multiple crystallographic sites. In this work, we investigate the thermometric behaviour of Nd^{3+}-doped yttrium fluoride (YF_3) and oxyfluoride ($Y_7O_6F_9$), by combining synchrotron X-ray diffraction, optical spectroscopy, and atomistic modelling. The structural evolution from YF_3 to $Y_7O_6F_9$, induced by oxygen incorporation, leads to the formation of multiple non-equivalent yttrium sites with distinct local coordination environments. Despite this structural complexity, the luminescence intensity ratio (LIR) approach based on Boltzmann statistics remains valid, yielding a threefold increase in relative sensitivity (from 0.22 to 0.68% K^{-1}). Atomistic simulations reveal that Nd^{3+} ions preferentially occupy specific crystallographic sites with similar local symmetry, effectively reducing the system to a dominant spectroscopic environment. Additionally, the incorporation of oxygen enhances the crystal field strength, increasing Stark level splitting and directly impacting the thermometric response. These results provide a physical basis for the observed luminescent behaviour and demonstrate how structural modifications govern thermometric performance in complex host matrices. This work establishes a structure–property framework that can guide the design of rare-earth-based luminescent thermometers beyond idealized single-site systems.

Keywords: Crystal filed effect, Nd-doped $Y_7O_6F_9$, Luminescent Thermometry.

K-06. Laser-patterned direct-write afterglow coatings for road safety

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Limited visibility remains a critical factor in night-time safety across transport and infrastructure systems, where conventional solutions rely heavily on external power sources or reflective geometries that are not always effective under real-world conditions. Persistent luminescent materials offer an alternative: passive light emission sustained for hours after excitation, without the need for continuous energy input.

In this presentation we introduce Direct-Write Afterglow on Standard Surfaces (DARS), a laser-driven approach that enables the in situ synthesis and patterning of persistent luminescent coatings directly onto functional substrates. By using power and position controlled laser, both material formation and spatial structuring are achieved in a single step, allowing robust, well-adhered luminescent features to be integrated onto a wide variety of surfaces. The laser-driven synthesis approach further enables localized defect engineering. The formation of trapping centers and activator environments can be controlled by tuning parameters such as energy density and thermal gradients, thus allowing modulation of emission intensity and decay dynamics through processing rather than composition alone.

The presented work demonstrates how laser-driven materials processing can bridge the gap between the research of advanced luminescent materials and real-world deployment, enabling practical, durable, and energy-efficient visibility solutions.

Figure 1: *A persistent luminescent pattern embedded directly on aluminum surface.*

This work is supported by OSI_PIP_BioPhoT-2025/2-0039 - DARS (Direct-write Afterglow on Standard Road Signs).

Keywords: persistent luminescence, optical materials, functional coatings.

K-07. Growth and characterization of rare-earth doped fluorite luminescent crystals

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In this work, the growth and structural and spectroscopic characterization of CaF_2 and BaF_2 crystals doped with several trivalent and divalent rare-earth ions (Tm, Tb, Ce, Er, and Yb) ions are investigated with the aim of developing efficient UV-VIS luminescent materials. High-quality single crystals were grown using the vertical Bridgman technique in the Crystal Growth Laboratory of the Faculty of Physics and Mathematics, West University of Timișoara. The crystalline quality of the obtained samples were evaluated through optical microscopy and etch-pit analysis, revealing a relatively low dislocation density on the order of ~10^3 cm^{-2} and a quasi-uniform distribution of dopant ions along the growth axis. Such characteristics indicate favorable growth conditions and good incorporation of rare-earth ions within the fluorite lattice. Optical absorption and photoluminescence measurements were performed to investigate the spectroscopic properties of the doped crystals. The spectra reveal characteristic electronic transitions associated with trivalent RE ions as well as the presence of divalent centers formed through valence conversion processes in the fluorite matrix. The radiative properties of the trivalent RE ions were further analyzed using the Judd–Ofelt formalism, enabling the determination of intensity parameters, radiative transition probabilities, branching ratios and radiative lifetimes relevant for evaluating the potential of these materials as laser active media. In addition, double-doped fluorite crystals containing trivalent and divalent RE ions were investigated. These systems exhibit emission bands in both the ultraviolet and visible spectral regions, suggesting efficient energy transfer processes between the sensitizer (Yb^{3+}) and the activator (Er^{3+}) ions. Such interactions are particularly relevant for the design of solid-state laser materials and upconversion-based photonic devices. Furthermore, dielectric spectroscopy measurements revealed relaxation processes associated with dipolar defect centers and charge-compensation mechanisms induced by aliovalent substitution of rare-earth ions in the fluorite lattice. The correlation between structural defects and dielectric response provides additional insight into the defect chemistry of rare-earth-doped fluorite crystals.

Keywords: rare-earth ions, luminescence, fluorite crystals.

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K-08. ERC Grants: From funding opportunities to proposal evaluation

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The European Research Council (ERC) funds frontier research based on scientific excellence and offers unique opportunities for researchers at different career stages. At the same time, preparing a competitive ERC proposal requires a good understanding of the funding schemes, evaluation process and reviewers' expectations.

This presentation will provide an overview of the ERC grants, explain the main evaluation steps and discuss practical aspects such as eligibility, panel choice and proposal preparation. It will also highlight common mistakes and share useful tips that can help applicants strengthen their proposals while remaining true to their own scientific vision.

The session is intended for researchers interested in applying for an ERC grant and aims to make the process more accessible, transparent and easier to navigate.

K-09. Luminescence of defects and isoelectronic impurities in UV-emitting oxide scintillators under X-ray and synchrotron radiation excitation

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Cationic isoelectronic impurities (CIIs) in oxide compounds, with respect to host cations of the same charge state, can efficiently localize low-energy excitations (electrons, holes, or excitons) by forming a non-Coulombic potential at the substitution site. For this reason, CIIs are widely used in the development of luminescent and scintillation materials operating in the UV spectral region, with good thermal stability at room temperature (RT).

This work is devoted to the analysis of the regularities governing the formation of luminescence centers associated with CIIs in $A_3Al_5O_{12}$ (A=Y, Lu) garnets doped with La^{3+} and Sc^{3+} ions. A similar approach is applied to antisite defects (ADs) in garnets, where Y^{3+} and Lu^{3+} ions occupy Al^{3+} sites in YAG and LuAG hosts, respectively. These defects can be considered as a specific type of CII [1]. Such ADs typically appear in 0.05–0.25 at.% content during the growth of garnet single crystals (SCs) from the melt at high temperatures (1900–2000 °C). In contrast, single crystalline films (SCFs) of these garnets grown by liquid-phase epitaxy are essentially free of ADs due to the much lower (~950–1050 °C) crystallization temperature. Therefore, SCs and SCFs of (Y, Lu)AG garnets represent useful model systems for studying the radiative relaxation of low- energy excitations, in particular exciton luminescence associated with CII and AD centers.

The investigation of the luminescent properties and electronic structure of CIIs in dielectric matrices is, however, challenging, since these impurities usually do not exhibit intra-center transitions in the UV–visible spectral range detectable by conventional absorption or luminescence spectroscopy. An effective approach is vacuum ultraviolet (VUV) luminescence spectroscopy under synchrotron radiation (SR) excitation, as employed in the present study.

The luminescence properties, including energy transfer processes from YAG and LuAG hosts to emission centers associated with CIIs and ADs, were studied using conventional spectroscopic techniques: cathodoluminescence at RT, X-ray-excited and tunneling luminescence spectra, as well as thermally stimulated luminescence (TSL) spectra and glow curves in the 80– 600 K temperature range. In addition, time-resolved luminescence measurements of SCs and SCFs of undoped as well as La^{3+}- and Sc^{3+}-doped YAG and LuAG were performed at the VUV station at the PETRA III storage ring (DESY, Germany) under pulsed SR excitation in the 3.7–12.5 eV range. This energy range covers part of the transparency region, the excitonic absorption region, and the onset of interband transitions in the host materials. Based on the obtained results, the energy structure of excitons localized at and bound to ADs as well as La^{3+} and Sc^{3+} CIIs in YAG and LuAG has been determined and competed with other dielectric materials doped with cation IIs.

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Keywords: Scintillators, luminescence, garnets, isoelectronic dopants, synchrotron radiation
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K-10. Radiation hardness of scintillation materials with high effective atomic number

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Hf-based and Gd-based scintillators such as Cs_2HfCl_6(CHC), Ce:$Gd_3(Al, Ga)_5O_{12}$ (Ce:GAGG) and Ce:$(La, Gd)_2Si_2O_7$ (Ce:La-GPS) have relatively higher light outputs and better energy resolutions (e.g. better than 5-7% at 662 keV, FWHM) [1-2] compared to conventional scintillators. These scintillators are expected to be used in several fields such as medical imaging, high energy physics and astronomy, and radiation hardness is one of the important factors under the high dose conditions (e.g. a satellite experiment conducted in earth orbit). In this paper, we grew CHC, Ce:GAGG and Ce:La-GPS crystals by the Bridgeman or Czochralski process and studied their radiation hardness.

These samples were irradiated with 80-MeV proton rays (current rate: ~0.01A, total dose: ~200 Gy) at the cyclotron faculty at Tohoku University. The range of 80-MeV protons in the Ce:La-GPS sample, for example, was estimated to be 17 mm from the calculation result of the SRIM code. Thus, 2 samples with sizes of 15 mm × 15 mm ×15 mm were prepared as shown in Fig. 1. Here, the one sample irradiated with proton beam was located at the plateau region of the Bragg curve (upstream side of the proton beam) and the other was corresponding to Bragg peak position (downstream side of the proton beam) to estimate the dependence of dE/dx for the scintillation properties.

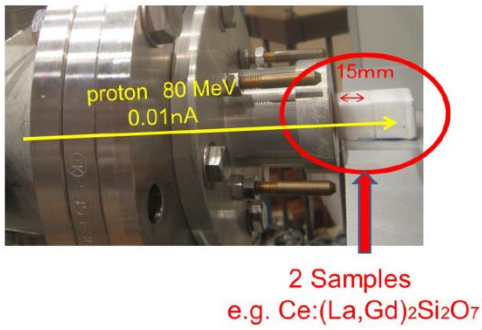

Figure 1: *Photograph of the setup for the proton irradiation into the Ce:La-GPS samples.*

The results show that light output and energy resolution remained constant before and after 80-MeV proton irradiation (~200 Gy). Additionally, the emission spectrum was the same as before irradiation, and no new emission peak originating from defects induced by the high-energy proton was observed. On the other hand, scintillation decay times were ~90 and ~ 130 ns before and after the irradiation, respectively. This paper reports the details of the results and discussion.

Keywords: keyword one, keyword two, keyword three.

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Invited speakers -abstracts-

I-01. Impact of impurity doping on vacancy type defects in functional materials revealed by positron annihilation spectroscopy

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Positron annihilation lifetime spectroscopy (PALS) is a unique experimental method used to identify vacancy-type defects in solids. This method is particularly effective for investigating the impact of impurity doping on vacancy-type defects in functional materials. We have performed PALS experiments using a radioisotope, a slow positron beam and ultrashort gamma-ray pulses for opto- and thermoelectric, and dielectric materials. In this talk, we present the impact of Mg and Sb ions on vacancy-type defects in multicomponent garnet scintillators and Kankyo semiconductors, respectively, as studied using PALS experiment.

The scintillation properties of multicomponent garnet oxides such as $Gd_3Al_2Ga_3O_{12}$:Ce have been reported to be drastically improved by Mg codoping. The impact of Mg codoping on improving scintillation properties has attracted significant attention. The PALS experiment revealed that the Mg codoping suppresses vacancy-type defects. Additionally, antisite defects, which are responsible for shallow electron traps, were remarkably reduced by the Mg codoping. This is because Mg atoms replace Al/Ga vacancies at the 16*a* and 24*d* sites, thereby eliminating the non-stoichiometric composition. Similar phenomena were observed with $Y_3Al_2Ga_3O_{12}$:Ce and $Lu_3Al_5O_{12}$:Ce, indicating that the Mg co-doping is a common feature of multicomponent garnet scintillators.

Mg_2Sn is a representative example of an environmentally friendly semiconductor, also known as a “Kankyo semiconductor”, consisting of abundant elements and having a low environmental impact. This material has been studied for potential applications in thermoelectric devices. Controlling native defects such as vacancies and interstitials is essential because they affect change carrier concentration and thermal conductivity, thereby impacting the figure of merit *ZT* for thermoelectric properties. Sb doping is known to improve the thermoelectric properties of Mg_2Sn. The PALS experiment demonstrated that Sb doping introduces Mg vacancies to compensate for the charge of Sb atoms at the Si site. The positron annihilation coincidence Doppler broadening spectroscopy (CDBS) experiment clarified that Sb atoms are distributed at a relatively high concentration around Mg vacancies. The Sb doping promotes the formation of nanoscale regions consisting of Sb atoms and Mg vacancies, resulting in improved *ZT*. The atomic arrangement in such nanoscale regions would be the same as the metastable cubic phase of Mg_3Sb_2 recently predicted.

Keywords: vacancy-type defects, PALS, multicomponent garnet scintillators, Kankyo semiconductors, impurity doping.

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I-02. Oxygen defects and ferroelectricity of $BaFe_{12}O_{19}$ hexaferrites

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The future of energy technologies extends beyond energy production to include energy storage, including batteries, fuel cells, and new supercapacitors. The latter are defined by the fast charging and discharging cycles necessary to provide pulsed current or voltage. Among them, the efficient electrostatic solid-state supercapacitors are based on ferroelectrics [1].

Recently, hexaferrite-based oxides with M=barium and strontium, having the complex formula $MFe_{12}O_{19}$, exhibit good ferroelectricity [2, 3], but this ferroelectricity is inhibited by oxygen defects that systematically reduce their polarizability [4]. The present paper describes the $BaFe_{12}O_{19}$ hexaferrites produced by the sol-gel technique, highlighting the role of oxygen vacancies and how they reduce ferroelectricity.

$BaFe_{12}O_{19}$ was thermally sintered at 1200°C for 4 hours followed by calcination in oxygen atmosphere at 800°C for 3 hours. The presence and evolution of oxygen defects were monitored using dielectric spectroscopy, thermoluminescence, and X-ray photoelectron spectroscopy to confirm their role as the dominant mobile ionic species.

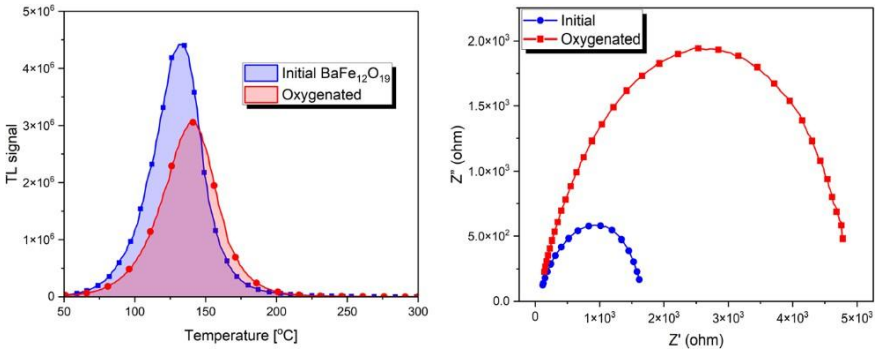

Figure 1: *Thermoluminescence and dielectric measurements.*

The reduction of the oxygen vacancies potentially decreases the density of the recombination centers, improving the ferroelectricity and the bandgap of the $BaFe_{12}O_{19}$.

Keywords: oxygen defects; barium hexaferrite; ferroelectricity.

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I-03. LGYSB:Nd crystal: Czochralski growth, optical properties, and NIR laser emission performances

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Incongruent melting $La_xNd_yGd_zY_wSc_{4-x-y-z-w}(BO_3)_4$ - LGYSB:Nd crystals with different Y concentrations (w = 0.15, 0.05, and 0.025) have been grown for the first time by the Czochralski method. For all crystals, the Nd^{3+} doping concentration in the starting melt composition was chosen to be 5 at.% (y = 0.05). Due to the peritectic nature of $La_xNd_yGd_zY_wSc_{4-x-y-z-w}(BO_3)_4$ compounds, which follow the stoichiometric composition (x + y + z + w = 1), a scandium deficiency (Sc < 3) is required in the starting melt composition to facilitate Czochralski growth of trigonal (space group *R32*) LGYSB:Nd-type crystals. Three initial melt compositions were tested, namely $La_{0.628}Gd_{0.422}Y_{0.15}Nd_{0.05}Sc_{2.75}(BO_3)_4$, $La_{0.628}Gd_{0.522}Y_{0.05}Nd_{0.05}Sc_{2.75}(BO_3)_4$, and $La_{0.628}Gd_{0.547}Y_{0.025}Nd_{0.05}Sc_{2.75}(BO_3)_4$ – LGYSB:Nd_3, respectively. The grown LGYSB:Nd_3 laser crystal operated at the emission wavelength of 1062 nm with very high slope efficiencies of η_{sa} = 0.74 and η_{sa} = 0.64 in quasi-CW (Fig. 1a) and CW (Fig. 1b) regimes, respectively, thus demonstrating its outstanding properties to generate efficient laser emission in the near-infrared (NIR) range [1].

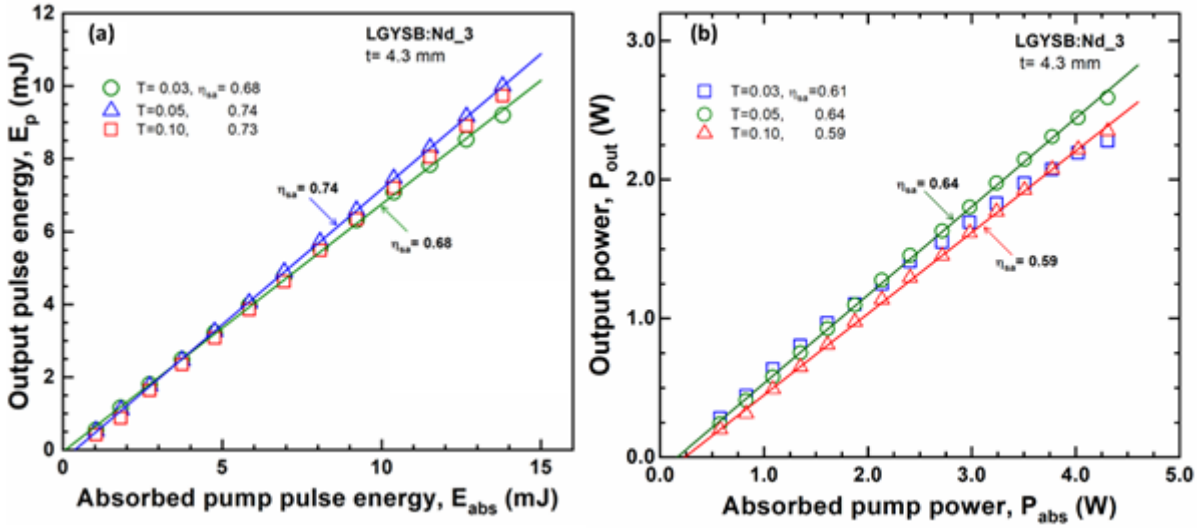

Figure 1: *Laser pulse energy, Ep versus absorbed energy of the pump pulse, E_{abs} (a), and output power, P_{out} versus absorbed pump power, Pabs (b) for LGYSB:Nd_3 crystal. T = transmission of output coupling mirrors and t = thickness of laser active medium.*

Keywords: Czochralski, nonlinear optical crystal, laser crystal.

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I-04. The role of structural defects caused by irradiation on the change in the properties of ceramic materials – promising materials for nuclear energy

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Interest in the use of ceramic materials in nuclear power is driven by the need to extend the service life of structural and functional materials capable of operating under extreme conditions and subject to high radiation doses. In nuclear reactors, materials are subjected to a combination of intense neutron and ion irradiation, high temperatures, thermoelastic stresses, and aggressive chemical environments. All of this leads to defect accumulation, structural degradation, and deterioration in the performance characteristics of traditional materials. Ceramic materials, thanks to their high temperature resistance, chemical inertness, radiation resistance, and low creep, are considered a promising alternative to metal alloys in a number of applications. They exhibit high oxidation stability, low thermal deformation, and the ability to maintain mechanical strength at elevated temperatures, which is particularly important for reactor core components and heat removal systems. This paper presents the key results of a series of experimental studies aimed at studying the mechanisms of defect formation in the near-surface layers of ceramic materials caused by ion irradiation at various temperature conditions. The studies identified the key stages in the evolution of structural damage in oxide ceramics and determined the mechanisms of irradiation-induced crystal structure destabilization depending on the irradiation dose.

Keywords: radiation damage, ceramics, structural materials, degradation of structural features.

I-05. SMART Growth: Artificial intelligence enhanced for sustainable growth of rare-earth materials based laser

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Crystal growth, by Czochralski method [1] for instance, for industrial photonics applications, is one of the crucial technologies for a modern society. Their manufacturing technology involves rare materials, high amount of energy, and a lot of dedicated process knowledge. The crystal, as a product itself, is a core component of many photonics systems such as the broad field of lasers for various applications. Nevertheless, the value chain for crystal growing is rarely based on Zero-Defect Manufacturing approaches that could enable a sustainable implementation of this crucial process.

SMART Growth project aims at developing single crystals for lasers and photonics applications under the supervision of Artificial Intelligence. Detecting, predicting and preventing failures in a typical crystal growth process are the key points for improving the yield of crystal production, reducing the amount of energy required and improving the quality of the as-grown crystal.

We present a study that integrates machine learning with numerical modeling. The objective is to unravel the nonlinear relationship between crystal growth process parameters and furnace geometry on one side, and solid/liquid interface shape and v/G (growth rate over temperature gradients) on the other side. We exemplify this approach by focusing on defect-free YAG and Ge crystals [2].

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Keywords: crystal growth, artificial intelligence, optical crystals

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I-06. Technology aspects of high-entropy oxides preparation by metalorganic aerosol deposition

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High-entropy oxides (HEO), containing five transition metals (Cr, Mn, Fe, Co, Ni) are an emerging class of materials with unique, tunable and stable physical properties (optic, magnetic, catalytic, electric etc.). Most of the oxides of these metals are good microwave absorbers due to their permeability. Thus, their direct use in coatings having various applications are foreseen. The synthesis of single-phase spinel HEOs - in particular, those using Cr, Mn, Fe, Co, and Ni - is challenging due to phase separation and site-distribution preferences driven by crystal-field effects. A chemical deposition technique, namely Metalorganic Aerosol Deposition (MAD) is employed due to its scalability and low cost. An aerosol of organic solutions containing β-diketonates precursors dissolved in dimethylformamide is sprayed with a precision pneumatic nozzle onto a heated substrate. The film growth is a result of a heterogeneous pyrolysis reaction owing to decomposition of the metal-organic precursors [1, 2]. Tailoring the concentration of these precursors allows the control over the thin film's composition.

MAD was successfully tuned for preparation of polycrystalline $(FeCoNiCrMn)_3O_4$ films on SiO_2/Si and epitaxial films on Al_2O_3 (0001) substrates aiming equimolar distribution of transition metals. Complex experimental analysis have been carried out by X-ray diffraction, XPS, EDX, SEM, TEM, KP and PYS. All the HEO films are spinel single phased with near-equimolar element distribution. Epitaxial films are single oriented out of plane revealing twinned-textured structure. Density of states and TEM reveal new insights on the functional properties of the HEO.

Keywords: High-entropy oxides, Metalorganic Aerosol Deposition, Defects.

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I-07. Characterization of oxygen-related Frenkel defects induced by energetic neutrons or ions in functional metal oxides

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Increasing radiation damage limits the use of functional materials operating under harsh radiation conditions, i.e., in the field of fission and projected fusion nuclear energetics. Thus, the mechanism of the creation of lattice defects (starting from elementary Frenkel ones) and damage recovery (via thermal annealing of irradiated crystals) is of special importance.

The radiation damage caused by fast fission neutrons or ~MeV-GeV swift heavy ions has been studied in α-Al_2O_3, MgO and $MgAl_2O_4$ wide-gap single crystals by means of optical absorption, EPR and cathodoluminescence methods [1-6]. The correlation between the EPR and optical characteristics (emission/absorption bands) has allowed to track the creation, transformation, accumulation, and further isochronal thermal annealing of classical *F*-type defects (an oxygen vacancy with one or two trapped electrons) [2-6] and more complex cation- containing defects [2, 3]. Notable that just an isolated (single) oxygen interstitial (to date detected only in neutron-irradiated corundum [1]) act as a mobile component in a temperature- stimulated recombination with the complementary *F* and F^+ centers in irradiated metal oxides.

The ion-fluence dependence of the concentration of oxygen-related Frenkel defects (estimated via optical or paramagnetic absorption) confirms their radiation origin (for the first time in case of charged and neutral interstitials in corundum crystals) [4]. The experimentally measured annealing kinetics of the *F* and F^+ (via integral of an optical absorption Gaussian or a relevant EPR signal) in metal oxides has also been modelled in terms of diffusion-controlled recombination reactions [1, 5, 6]. In α-Al_2O_3 and MgO irradiated either by energetic neutrons or ions, the features in several EPR characteristics of the F^+ and O^- (involves a charged oxygen interstitial) Frenkel defects and in the annealing kinetics of the oxygen-vacancy-containing *F* and F^+ centers have been revealed$_2$ and discussed [5]. The radiation-induced suppression of intrinsic luminescence as well as the limitations of the use of typical emission bands for the control over Frenkel defects in corundum have been considered [4].

Keywords: oxygen-related Frenkel defects; irradiation by energetic ions or neutrons; optical and paramagnetic absorption.

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I-08. Reading without erasing: A study of trapped charges in radiochromic and radio-photoluminescence phosphors

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Passive radiation dosimeters with thermoluminescence or optically stimulated luminescence read-out are well known and among the most sensitive radiation detector materials. However, the dose information, which is stored in these materials as radiation-induced electrons and holes trapped at defects, is erased during read-out [1,2]. As an alternative, we investigated phosphors that are sensitive to UV and shorter-wavelength ionizing radiation, with optical read-out schemes that do not involve charge-carrier detrapping, in particular radiochromic (RC) [3] and radio-photoluminescent (RPL) phosphors [4,5]. The RC phosphors rely on the formation of intrinsic color centers. In the RPL phosphors we studied, electron capture by Eu^{3+} dopant ions results in the formation of stable Eu^{2+} centers, leading to a change in the photoluminescence (PL) emission color. The Eu^{2+}/Eu^{3+} PL intensity ratio thus serves as a self-referenced indicator of the absorbed dose.

In this presentation, results from our combined optical and electron paramagnetic resonance (EPR) spectroscopic studies of these phosphors will be presented. The aim is to identify the trapped electron and hole states involved in radiation information storage as well as in the optical read-out signal. In the RC phosphor, we were able to identify the charge states corresponding to the intrinsic defect's "bleached" and "colored" states. For Eu-doped Ba_2SiO_4 and $Ba_3(PO_4)_2$ RPL phosphors, PL and EPR measurements show that electron trapping at Eu^{3+} exhibits site-selectivity. Scanning electron microscopy measurements, combined with energy-dispersive X-ray spectroscopy and cathodoluminescence, assist in correctly interpreting the PL and EPR data.

Keywords: Radiation defects, Rare-earth dopant, Radiochromism, Radio-photoluminescence.

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I-09. Morphology-controlled Er-doped ZnO nanorods with enhanced NIR emission and defect modulation

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Erbium-doped ZnO powders with Er concentrations of 1, 2, and 5 at.% were synthesized via a hydrothermal method and systematically characterized for their structural, morphological, textural, optical, and magnetic properties. X-ray diffraction (XRD) confirmed the formation of a hexagonal wurtzite ZnO phase (space group P63mc) with lattice parameters a ~ 3.25 Å and c ~5.21 Å, showing minimal variation with increasing Er content, indicative of partial Er incorporation into the ZnO lattice. Transmission electron microscopy (TEM) revealed rod-like nanostructures with lengths of ~100–500 nm, consistent with preferential growth along the c-axis. Contrast variations suggest the presence of low-density or partially hollow interior regions. High-resolution TEM images exhibited clear lattice fringes with an interplanar spacing of ~ 0.26 nm, corresponding to the (002) plane, along with slight distortions attributed to Er-induced lattice strain. Selected area electron diffraction patterns showed well-defined concentric rings with discrete spots, confirming the polycrystalline wurtzite structure. Nitrogen adsorption–desorption isotherms (Type IV) indicated mesoporosity, with surface area increasing with Er content. Photoluminescence measurements revealed near-band-edge emission at ~380 nm and defect-related visible emission around 650 nm. Under 980 nm excitation, characteristic Er^{3+} emissions at ~1 µm and ~1.53 µm were observed. Electron paramagnetic resonance confirmed the presence of intrinsic defects and paramagnetic Er^{3+} ions, with defect passivation occurring at higher doping levels. Collectively, these results demonstrate that hydrothermal synthesis yields hollow Er-doped ZnO nanorods with tunable porosity, optically active Er^{3+} centers that emit in the NIR telecommunication window, and a systematically modifiable defect population, making these materials highly promising for photonic, sensing, and catalytic applications.

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I-10. Role of localized electronic levels in scintillating materials for high-energy radiation detection

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The detection of ionizing radiation is at the heart of many strategic applications in both science and technology, including high-energy/particle physics, space exploration, medical diagnostics, border security, and industrial and environmental monitoring. In all such areas, scintillating materials are frequently used, that convert the energy deposited by ionizing radiation into UV or visible photons, which are then easily detected by common photodetectors. Scintillation light originates from radiative transitions at intrinsic centers or dopants used as activators: therefore, a fast and efficient transport to the luminescent centers of carriers generated upon the interaction with ionizing radiation is fundamental in the scintillation process. The efficiency and speed of carrier transfer through the host matrix are affected by the presence of defects, leading to trapping levels in the forbidden energy gap, which can temporarily capture migrating charge carriers, either delaying their radiative recombination at emission centers or decreasing the overall scintillation efficiency. Experimental investigations on traps are aimed at finding their characteristic parameters, like the thermal depth, the frequency factor, and the order of kinetics, that enable to predict their lifetime at a given temperature and, consequently, their expected influence on the scintillation process. Sometimes, also the microscopic nature of such defects can be disclosed. Therefore, the study of the characteristics and role of defects in the scintillation mechanism becomes essential in the science of scintillators and has seen significant progress in the recent years, extending from inorganic single crystals to glasses, ceramics, and hybrid systems like semiconductor nanocrystals, and polymeric nanocomposites.

Several studies were devoted to single crystalline scintillators that usually show well-localized intragap electronic levels; in contrast, an in-depth analysis of the role of point defects and of their close interplay with luminescent activators in the recombination processes governing the scintillation emission is not commonly encountered concerning amorphous materials, such as silica, due to the difficulty of disentangling trap levels subjected to inhomogeneous broadening. On the other hand, polycrystalline ceramics and nanocrystals are recently emerging as promising new classes of scintillating materials; however, despite their potential, as of today, few examples tackled in depth the mechanism leading to scintillation light, as well as not much is known on the details of trapping and detrapping processes involved in their scintillation emission.

In this context, I discuss an effective approach based on the combination of thermally stimulated luminescence, temperature-dependent steady-state and time-resolved radioluminescence for the investigation of the role of trapping sites in scintillating materials and for the determination of the effects of long-term and high dose ionizing radiation exposure. Specifically, the results obtained on various classes of materials are outlined, moving from amorphous silica and bulk crystals to polycrystalline garnet ceramics and nanostructured materials.

Keywords: scintillation, traps, thermally stimulated luminescence.

I-11. The impact of structure and composition on fast-emitting lightweight hybrid scintillators

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Scintillators down-convert ionizing radiation into UV/visible light, with efficiency governed by atomic number Z and density. They are key in biomedical applications such as time-of-flight positron emission tomography (ToF-PET) for high-resolution imaging and X- ray-induced photodynamic therapy (X-PDT), where scintillation activates photosensitizers to generate cytotoxic species.

Recently developed, hybrid scintillators combine high-Z components with fast-emitting organic materials to achieve both efficient radiation interaction and rapid emission. We focus on two classes: (i) scintillating composites of UV-emitting polymer matrices with dense high- Z nanoparticles and high-quantum-yield fast dyes, and (ii) Metal-organic framework (MOF) composed by high-Z linking nodes and emissive ligands, offering a tuneable crystalline architecture. X-ray interactions with these nanostructured systems generate secondary charges whose density and tracks govern the formation of excitons that travel towards the final emissive states. [1-2] Charges can be trapped by defects or quenching centres, and in diffusive crystalline systems, excitons may access these sites, leading to non-radiative losses and slower emission kinetics.

In scintillating composites, performance depends on the compatibility and energy alignment of the polymer host, nanoparticles, and fluorescent dyes. Fine-tuning these properties enhances charge recombination and energy transfer, minimizes quenching, and produces highly luminous nanocomposites. [3] In MOFs, scintillation is dictated by the interplay between metal nodes and ligands: ligand–node matching, crystallinity, and topology rule exciton diffusion and ultrafast processes, ensuring fast and efficient emission. [4]

This work shows that optimizing structural organization, composition, and charge transport is essential to suppress non-radiative losses and enhance both light yield and timing response. By engineering component properties in composites and controlling node–ligand interactions in MOFs, we can establish a versatile platform for next-generation scintillators with tailored optical and timing properties for advanced biomedical imaging and radiation- based applications.

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I-12. 2D MoS_2 from thermal stability to irradiation induced modifications

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The emerging interest on single atomic thickness materials (2D-materials) in all their electronic configurations (insulator, semiconductor, metal) pushes for the better understanding of their native features as well as their stability by irradiation or by thermal processing. Among the members of this family, 2D transition metal dichalcogenides (2D-TMD) and in particular MoS_2 are of particular concern for their application in frontier semiconducting devices. Furthemore 2D-MoS_2 features a direct bandgap of about 1.8 eV associated to an excitonic emission that is exploitable for optoelectronic applications.

In this work we compare monolayers of MoS_2 produced by bottom up (Chemical Vapor Deposition) and top-down (mechanical exfoliation) methods and transferred on insulating (SiO_2), semiconducting (GaN) and metallic (Au) substrate highlighting their electronic and optical features. The effects of electron irradiation are then considered evidencing that sulfur vacancies could be induced affecting the doping of the material depending on the electron energy and dose [1-2]. Finally the thermal stability of the material is considered in a temperature range below 350°C evidencing that a controllable tuning of doping and of emission features can be obtained [3]. Overall, the reported results shed new light on the application of 2D-MoS_2 and its post growth modifications as well as its exploitability in harsh environments.

Keywords: Monolayer MoS_2, β-ray irradiation, Thermal processing.

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Oral presentations -abstracts-

O-01. Electronic and optical properties of YVO_4:Eu induced by different charge states of the Eu ion: an ab-initio study

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$YVO_4:Eu^{3+}$ is a well-known red phosphor [1], widely used in a variety of optical devices [2,3]. Its red emission stems from f–f transitions of Eu^{3+}, specifically from the excited $^5D_0$ state to the ^7F_J (J = 0–4) manifold, resulting in sharp emission lines around 600 nm [2]. Although these transitions are largely host-independent, the emission properties can be modified by gamma irradiation, as demonstrated in a recent experimental study [4]. In the latter, the authors reported suppression of the characteristic Eu^{3+} sharp emission peaks and the emergence of a broad emission band around 470 nm, attributed to the partial reduction of Eu^{3+} to Eu^{2+}. Consequently, gamma irradiation induces a shift in emission from the red to the blue region, opening possibilities for tunable phosphor applications.

In this work, we simulate the effects of gamma irradiation on $YVO_4:Eu^{3+}$ using Density Functional Theory (DFT). Gamma irradiation ejects some electrons from the material's interior, which may be captured by Eu^{3+} ions, potentially altering their charge state. First, we perform DFT calculations for pristine $YVO_4:Eu^{3+}$, carefully calibrating the electronic structure to reproduce the experimentally observed optical absorption [4]. We then model the irradiated system by introducing one additional electron into the $YVO_4:Eu^{3+}$ unit cell and compare its electronic and optical properties with those of the neutral system. Our results show that Eu^{3+} captures a significant fraction of the additional charge (~0.32e), although this is insufficient to confirm a full reduction to Eu^{2+} oxidation state. Nevertheless, the Eu-related electronic structure undergoes substantial changes: the occupied 4f states shift to higher energies and move closer to the conduction band minimum, where Eu 5d states are located. As a result, the dominant optical transitions change from intraband (f–f) in the neutral system to interband f–d transitions in the charged system. These findings explain why the emission spectrum of non-irradiated $YVO_4:Eu^{3+}$ consists of sharp, discrete peaks, whereas gamma-irradiated samples exhibit a broad emission band, which is sensitive to the crystal field and can be tuned.
Detailed results are reported in Refs. [5,6].

Keywords: red phosphor; electronic structure; optical absorption

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O-02. Swift heavy-ion induced defect formation and luminescence modification in Ce-doped garnet single crystalline films

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Cerium-doped garnets $R_3Al_5O_{12}$:Ce (R = Lu, Y) are widely used as scintillation and dosimetric materials due to their high light yield and fast response. Their radiation stability is strongly influenced by structural defects, including antisite defects and oxygen vacancies, which are typically present in bulk melt-grown crystals. In contrast, single crystalline films (SCFs) grown by liquid-phase epitaxy under oxygen-rich conditions exhibit near-stoichiometric composition and reduced defect concentration, making them suitable model systems for studying intrinsic radiation tolerance.

In this work, the influence of swift heavy-ion irradiation on structural and luminescent properties of $Lu_3Al_5O_{12}$:Ce and $Y_3Al_5O_{12}$:Ce SCF scintillators was investigated. Samples were irradiated at 300 K with 147 MeV ^{84}Kr ions to fluences of 10^{12} and 10^{14} ions/cm² using the DC-60 accelerator (Astana, Kazakhstan). Radiation-induced modifications were analyzed using Raman spectroscopy, optical absorption, cathodoluminescence (CL), photoluminescence (PL), scintillation light yield (LY), decay kinetics measurements, and UV–VUV spectroscopy (3.7–12.5 eV) under synchrotron excitation at 13 and 300 K at the P66 beamline of PETRA III (DESY, Germany).

Pronounced changes in structural and luminescent characteristics were observed at the fluence of 10^{14} ions/cm². These modifications are attributed to the formation of radiation-induced point defects and latent ion tracks, as confirmed by absorption, CL, and PL spectra. Track overlap effects begin near 10^{12} ions/cm², while higher fluences promote bond breaking within the garnet lattice. High electronic energy losses lead to strong local heating along the ion trajectory, stimulating the formation of self-trapped and localized excitons, antisite-related defects, and oxygen vacancies. Additional defect generation occurs near the ion end-of-range due to increased nuclear stopping.

Synchrotron-excited luminescence demonstrates distinct fluence-dependent behavior for Y- and Lu-based garnets. In YAG:Ce, excitonic excitation in the 6.9–7.8 eV range (13 K) significantly enhances emission from F^+ and F centers at the fluence of 10^{14} ions/cm², while this emission is suppressed at 300 K. In contrast, LuAG:Ce exhibits increased Ce^{3+} photoluminescence intensity, enhanced scintillation light yield, and decay kinetics approximately three times faster than in YAG:Ce. These results reveal different radiation response mechanisms in Lu- and Y-containing garnet SC

Keywords: Swift heavy-ion irradiation; Ce-doped garnets; Single crystalline films

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O-03. Development of Nd-doped LGSB crystals as new candidates for the next generation of bifunctional crystals

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Currently, many researches are focused on the development of new bifunctional laser and nonlinear optical (NLO) or on improving existing ones based on new concepts. Very recently, our group has developed Czochralski-grown $La_xGd_yNd_zSc_{4-x-y-z}(BO_3)_4$ (LGSB:Nd) bifunctional crystals, as very promising active media for the construction of highly efficient lasers in the near-infrared (NIR) domain, as well as compact visible (VIS) lasers based on self- frequency doubling (SFD) processes. Considering the incongruent melting of LGSB:Nd crystals, the starting melt compositions and the pulling and rotation rates were optimized. Also, a special thermal setup was engineered to grow LGSB:Nd-type crystals by the Czochralski crystal growth method. High optical quality LGSB:Nd crystals doped with various concentrations of Nd^{3+} ions (2.3, 3.5, and 4.6 at.%) were grown by the Czochralski method, for the first time, according to our knowledge [1]. The as-grown crystals are shown in Figure 1.

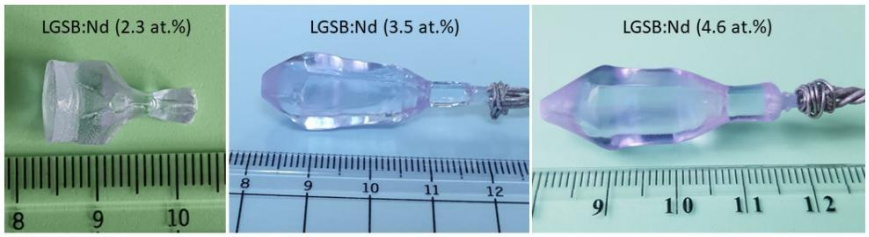

Figure 1: *Photos of Czochralski-grown Nd:LGSB-type crystals.*

The structural and optical properties of the grown crystals, as well as their laser performances, were evaluated. The obtained results demonstrate their favorable intrinsic properties for generating laser emission in the NIR domain (~1 µm) with very high efficiency. A high slope efficiency of 0.73 was obtained for the LGSB:Nd (4.6 at.%) crystal in quasi- continuous-wave (quasi-CW) operation. The main NLO properties of all grown crystals were found to be similar to those of the undoped LGSB crystal. Preliminary SFD experiments were also carried out. In the case of the LGSB:Nd (3.5 at.%) crystal, a green (~ 530 nm) SFD power of 48 mW was achieved.

Acknowledgement: This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0154, within PNCDI IV.

Keywords: crystal, laser, neodymium.

References:

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O-04. High-performance multi-wavelength laser emission from a newly developed Nd-doped LYSB crystal

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Incongruent melting Nd-doped $La_xY_ySc_{4-x-y}(BO_3)_4$ crystals were grown for the first time by the Czochralski method. The starting melt composition was optimized to reduce the defects in the grown crystal. The composition of the best-quality grown crystal was measured to be $La_{0.7830}Nd_{0.0398}Y_{0.3533}Sc_{2.8239}(BO_3)_4$. The Powder X-ray Diffraction revealed a trigonal single phase (space group *R32*). The spectroscopic properties of Nd^{3+} ions were investigated at room temperature and at 10 K. Laser experiments demonstrate multi-wavelength emission at 0.9 µm,
1.06 µm, and 1.3 µm in Nd:LYSB crystal, with slope efficiencies comparable to Nd:YAG and vanadate lasers, while offering the additional advantage of intrinsic nonlinear optical properties for second- and third-harmonic generation. The laser emission performance at λ_{em} = 1.06 µm is presented in Figure 1 under laser diode pumping at 808 nm and 880 nm.

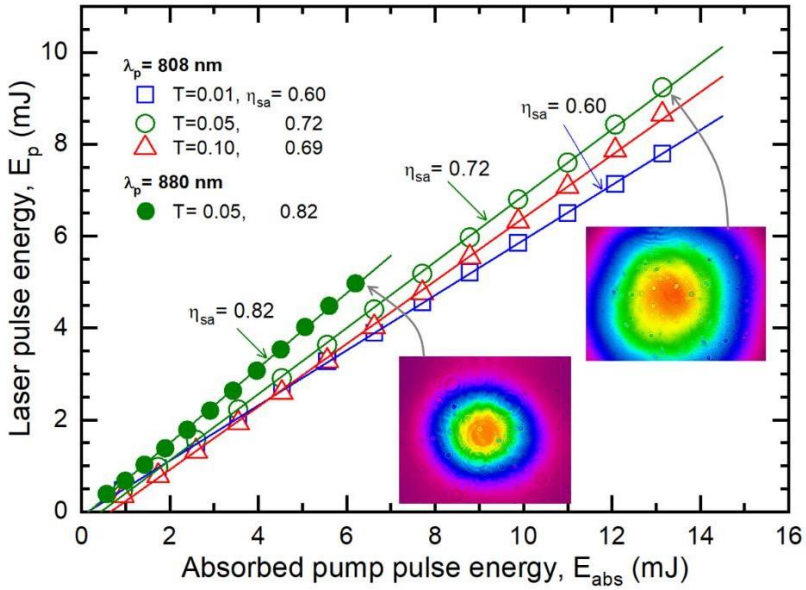

Figure 1. *Laser pulse energy (E_p) at 1.06 µm obtained from the Nd:LYSB crystal under pumping at 808 nm and 880 nm. Insets show the near-field beam profiles (2D intensity maps) at the indicated operating points.T denotes the output coupler mirror (OCM) transmission at 1.06 µm. Solid lines represent fits to the experimental data.*

Keywords: Czochralski, borate crystal, laser emission.

Funding: *This work was supported by a grant of the Ministry of Education and Research, CCCDI – UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0154, within PNCDI IV.*

O-05. Control of the emission wavelength of Cs_2HfCl_6 via tetravalent ion doping

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Near-infrared (NIR) light sources play an important role in a wide range of applications, including biological remote sensing, owing to their high penetration depth compared to visible light[1]. As promising phosphors, zero-dimensional halide Cs_2BX_6 (B: tetravalent ion, X: halide) perovskites such as Cs_2HfCl_6 have attracted considerable attention due to the high quantum efficiency arising from strong electron–phonon coupling and the formation of self-trapped excitons. Furthermore, compositional engineering such as substitution of halide ions in the valence band (e.g., substituting Cl^- with I^-) reduces the bandgap, enabling a redshift of the emission wavelength to the 650–700 nm range [2]. However, such iodide-based materials generally suffer from stability under ambient conditions. Therefore, in this study, we focus on substitution at tetravalent ion site of the vacancy-ordered halide Cs_2HfCl_6 as a host material.

Pt was selected as the dopant for the tetravalent ion. Pt -doped Cs_2HfCl_6 (Pt:CHC) were grown using the Bridgman- Stockbarger method. To evaluate the emission properties and mechanism, temperature dependences of photoluminescence (PL) spectra were measured at the BL3B beamline at UVSOR, the Institute for Molecular Science.

As shown in Fig.1, the crystal exhibited orange to red emission under UV irradiation. Figure 1 also shows the temperature dependence of the luminescence properties under excitation at 360 nm. Emission bands were observed at approximately 1.8 eV (low energy) which may be related to $[PtCl_6]^{2-}$. In this presentation, we will report on the detailed luminescence properties.

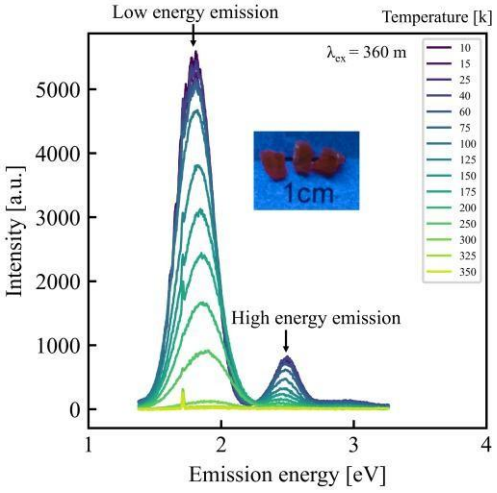

Figure 1: *Appearance of Pt:Cs_2HfCl_6 and temperature dependence of PL spectra*

Keywords: NIR phosphor, Halide perovskite, Optical materials.

References:

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O-06. Multi-spectroscopic studies of defects in quartz as a natural dosimeter

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Quartz contains a wide range of intrinsic (mainly oxygen-related) and impurity-associated defects (e.g., Al, Ti, Ge), some of which remain stable under ionizing radiation, while others transform. Paramagnetic defects—such as E' centers (≡Si·), peroxy centers (≡Si–O–O·), non-bridging oxygen hole centers (NBOHC, ≡Si–O·), and impurity-related centers ($[AlO_4]^0$, $[TiO_4^-/M^+]^0$, $[GeO_4]^0$)—can be detected by electron paramagnetic resonance (EPR). In parallel, luminescent defects such as NBOHC and oxygen deficiency centers (ODC, ≡Si–Si≡) are characterized by photoluminescence and cathodoluminescence. The dynamics of these radiation-sensitive defects allow quartz to act as a natural dosimeter, forming the basis of trapped charge dating methods including thermoluminescence (TL), optically stimulated luminescence (OSL), and EPR.

While OSL has been extensively applied for dating over the past decades, existing models largely neglect the role of ionic mobility within the quartz lattice, implicitly assuming that defect populations are static apart from electron trapping and recombination processes. In this study, we explicitly address this limitation by investigating the role of mobile ionic species and their interaction with defect structures under natural irradiation conditions.

We apply a multi-spectroscopic approach combining TL, OSL, EPR, and hyperspectral cathodoluminescence (SEM-CL) to quartz extracted from independently dated rocks of varying ages and their derived sediments from global environments. Our results support the hypothesis that intrinsic defects preserve genetic information related to quartz provenance, provided no metamorphic or high-temperature resetting has occurred. Furthermore, building on previous work, we show that OSL sensitization in nature is controlled by precursor defects linked to impurities such as Ti, but also significantly influenced by processes not reproduced in laboratory conditions.

We propose that ionic mobility plays a key role in evolution, redistribution, and amplification of defect structures in natural environments. Incorporating ionic mobility into defect models represents a critical step toward a more complete physical understanding of luminescence processes and strengthens the use of quartz as both a geochronometer and a provenance tracer.

Keywords: quartz defects, optically stimulated luminescence (OSL), ionic mobility, electron paramagnetic resonance (EPR), thermoluminescence (TL), cathodoluminescence.

Acknowledgement: This research is funded by European Research Council ERC grant PROGRESS-CoG "Reading provenance from ubiquitous quartz: understanding the changes occurring in its lattice defects in its journey in time and space by physical methods"

O-07. Mapping defect energy levels in Ce-doped $KMgF_3$ via synchrotron-based X-ray spectroscopy

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X-ray absorption spectroscopy (XAS) is widely used to probe the local electronic and geometric structure of solid-state materials. In lanthanide-doped systems, L-edge XANES and EXAFS are commonly employed to determine dopant valence and local coordination, often combined with optical techniques such as XEOL and UV–Vis to investigate luminescence mechanisms. However, aliovalent doping introduces charge-compensating defects that create electronic states within the bandgap, significantly affecting luminescence properties, such as lifetime, emission color, and trapping processes. A set of experimental, including thermoluminescence (TL), electron paramagnetic resonance (EPR), techniques have been applied to explain these issues. Furthermore, computational atomistic modelling can provide some insights about mechanisms before emission. Nevertheless, all these techniques are not element-selective and often rely on indirect interpretations. In this work, we employ a suite of synchrotron-based X-ray techniques to directly investigate defect-related electronic levels within the bandgap. Ce-doped $KMgF_3$ fluoroperovskite was used as a model system. Polycrystalline samples were synthesized via microwave-assisted hydrothermal methods and pre-characterized structurally and optically. By combining XAS, X-ray Photoelectron Spectroscopy (XPS), and Resonant Inelastic X-ray Scattering (RIXS), we construct an experimental electronic configuration scheme and critically compare it with empirical Host-Referred and Vacuum-Referred Binding Energy (HRBE/VRBE) models. Measurements were carried out on IPE beamline at LNLS under proposals 20250969 and 20250920 and LNNano laboratory under proposal 20252259. The combined spectroscopic analysis with DFT modelling demonstrates that element-selective X-ray techniques can resolve dopant- and defect-related electronic states providing a refined description of compensation mechanisms and improving current luminescence models. (Acknowledgment: this work was support by PCI-CNPQ 2025/2, CAPES, FAPESP and FAPITEC/SE).

Keywords: Ce-doped KMgF3, defect energy levels, X-ray techniques and DFT.

O-08. Structural and optical properties of YAG:Ce single-crystalline film phosphors under high-pressure and low-temperature conditions: impact of homo- and quasi-homoepitaxial growth

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Ce-doped $Y_3Al_5O_{12}$ (YAG:Ce) single-crystalline films (SCF) are widely used as efficient scintillating and phosphor materials; however, their performance is highly sensitive to strain state, defect structure, and epitaxial growth conditions. In particular, the role of lattice mismatch-induced strain and its coupling to optical centers under extreme thermodynamic conditions remains insufficiently understood. This work addresses the fundamental problem of how homoepitaxial (HE) and quasi-homo-epitaxial (QHE) growth modes influence the structural relaxation, defect formation, and optical response of YAG:Ce SCF under high pressure and low temperature. YAG:Ce SCFs were grown by liquid phase epitaxy (LPE) on YAG and LuAG substrates, corresponding to HE and QHE configurations, respectively. The lattice mismatch in the QHE system introduces internal mechanical stress, providing a controlled platform for studying strain–luminescence coupling. The structural, luminescence, and decay kinetics properties were investigated over a wide temperature range (12–500 K) and under high hydrostatic pressure up to 18 GPa using diamond anvil cell. X-ray diffraction analysis confirms full elastic relaxation in both systems, while revealing subtle anisotropic distortions reflected in differences between in-plane and out-of-plane lattice parameters.These structural perturbations lead to measurable modifications of the local crystal field around Ce^{3+} centers, resulting in shifts of 6–12 meV in the $4f–5d_{1,2}$ absorption bands and appr. 6 meV in the emission band energy between HE and QHE films. Temperature-dependent studies show a decrease in emission intensity for both systems, accompanied by pronounced changes in decay kinetics, suggesting defect-assisted non-radiative channels. The observed behaviour may be associated with the formation of Ce^{4+}–Pb^{2+} defect complexes during epitaxial growth. Under external pressure, both systems exhibit a non-monotonic redshift of the Ce^{3+} emission band (up to several tens of meV) and a pressure-induced reduction of decay time consistent with thermally activated (Boltzmann-type) relaxation processes. Importantly, the pressure response differs significantly between HE and QHE films, with distinct decay-time slopes (21–41 ns for YAG:Ce/YAG and 16–53 ns for YAG:Ce/LuAG), highlighting the role of epitaxial strain in governing electron–lattice coupling. Overall, this study demonstrates that HE and QHE growth modes critically determine the interplay between strain, defect structure, and luminescence dynamics in YAG:Ce SCFs under extreme conditions, providing new insight into strain-engineered control of optical functionality.

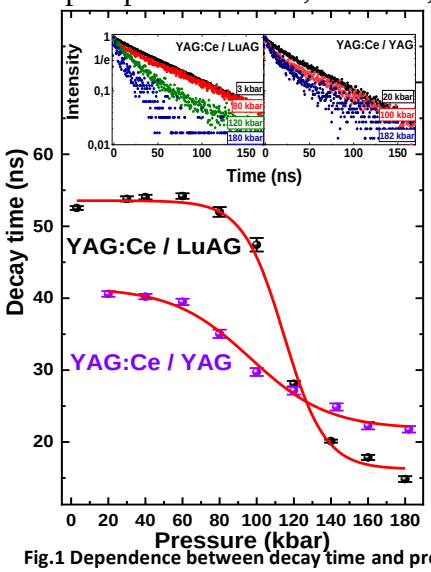

Fig.1 Dependence between decay time and pressure in the studied epitaxial structures under 430 nm

Keywords: Liquid phase epitaxy, single crystalline films, $Y_3Al_5O_{12}$, X-ray diffraction, Ce^{3+} ions, luminescence, high-pressure.

References: [1] A. Markovskyi at al, CrystEngComm 27 (2025) 256–268.

O-09. UV-VUV induced thermally stimulated luminescence in scintillating crystals using synchrotron radiation

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The detection of ionizing radiation is at the heart of many strategic applications in both science and technology, including high-energy/particle physics, space exploration, medical diagnostics, border security, and industrial and environmental monitoring. In all such areas, indirect detectors are frequently used, that include scintillating materials converting the energy deposited by ionizing radiation into UV or visible photons, which are then turned into electrical signals by coupled photodetectors.

Scintillation light originates from radiative transitions at intrinsic centers or dopants used as activators: therefore, a fast and efficient transport to the luminescent centers of carriers generated upon the interaction between ionizing radiation and the scintillating material is fundamental in the scintillation process. The efficiency and speed of carrier transfer through the host matrix are affected by the presence of defects, leading to trapping levels in the forbidden energy gap, which can temporarily capture migrating charge carriers, either delaying their radiative recombination at emission centers or decreasing the overall scintillation efficiency. Experimental investigations on traps are aimed at finding their characteristic parameters, like the thermal depth, the frequency factor, and the order of kinetics, that enable to predict their lifetime at a given temperature and, consequently, their expected influence on the scintillation process. Sometimes, also the microscopic nature of such defects can be disclosed. Therefore, the study of the characteristics and role of defects in the scintillation mechanism becomes essential in the science of scintillators and has seen significant progress in the recent years.

In this work, we report the analysis of trapping/de-trapping/re-trapping mechanisms in rare earth-doped garnet and perovskite single crystals by spectrally resolved thermally stimulated luminescence excited by synchrotron radiation in the 4 to 40 eV range collected at the P66-Superlumi end station of the DESY synchrotron facility in Hamburg, and its correlation with the spectrum of band-to-band electronic excitations.

The obtained results elucidate the close interplay between defects acting as trapping sites and the electronic levels of luminescent centers introduced in the host matrix as extrinsic activators. This study contributes to give an answer to the lack of fundamental knowledge about the electronic trapping and detrapping mechanisms responsible for radio- and thermo-luminescence, and to set an approach for the monitoring of the concentration of performance critical defects, inevitably present even in materials grown in the most controlled conditions.

Keywords: scintillation, carrier dynamics, thermoluminescence, synchrotron radiation.

O-10. Stability and synthesis attempt of novel A_2(Ce/Pr)WO_6 double perovskites (A=Ba, Sr, Ca) in the prospect of future energy conversion applications.

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Heavy-metal double perovskites have emerged as an important and intensively studied class of materials for applications in energy conversion and power-related technologies. Although most compounds in this family are insulating, a significant number exhibit semiconducting behavior, which has stimulated interest in their use in microwave dielectrics, piezoelectric sensors, and electrode materials for fuel and solar cells.

In this work, we explore the synthesis of novel double perovskite systems of general formula $A_2BB'O_6$, combining tungstate units (B' = $W^{4+/5+}$) with cerate or praseodymate units [B = (Ce or Pr)$^{4+/3+}$]. By varying the alkaline-earth A-site cation (Ba, Sr, or Ca)$^{2+}$, we aim to tailor the structural and electronic properties of the host lattice, with the long-term goal of developing efficient near-UV to near-IR down-conversion materials upon future doping with rare-earth ions such as (Yb, Eu, or Dy)$^{3+}$.

The obtained results reveal a strong dependence of crystal structure on the A-site cation. Ba-based compounds ($Ba_2Ce/PrWO_6$) crystallize as nearly cubic double perovskites (monoclinic, $I2/m$, $\beta \approx 90.4°$),[1,2] whereas the Sr-based system adopts a more complex quaternary perovskite structure ($Sr_9Ce_2W_4O_{24}$, tetragonal $I4_1/a$).[3] In contrast, Ca-based compositions form a non-centrosymmetric ilmenite-type structure ($Ca_3Ce_2W_2O_{12}$, rhombohedral R-3c).[1] These structural variations significantly impair host stability by charge-transfer processes, which, in turn, critically influence efficient and stable photoluminescence. To elucidate the underlying structure–property relationships, a combination of complementary characterization techniques was employed, including Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDX), scanning electron microscopy (SEM), differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA). Selected key findings from these methods will be highlighted, with particular emphasis on challenges related to structural stability and luminescence performance under excitation.

Keywords: Polymorphism, Double perovskites, Stability

References:

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Acknowledgement. "The financial support of the European Research Executive Agency (HORIZON-MSCA-2023-SE-01 Project No. 101182995) is acknowledged."

O-11. Luminescence dynamics of $CsPbI_3$ perovskite nanocrystal scintillators

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Scintillating nanoparticles have recently attracted significant attention as versatile alternatives to traditional bulk scintillators due to their tunable optical properties, fast response times, and the ability to be processed into polymeric composites. These nanoscale systems offer the possibility to tailor luminescence and scintillation properties through control of their structural, electronic, and chemical characteristics, including dimensionality and defect distribution [1]. Embedding nanocrystals in polymer matrices allows the fabrication of robust, easily processable materials that provide efficient light detection, while also offering environmental stabilization and reduced production costs [2]. Such composites are therefore particularly suited to the demanding requirements of modern technological and medical applications. Lead halide perovskite (LHP) nanocrystals have emerged as promising candidates for next- generation scintillators, combining high interaction cross-sections for ionizing radiation, fast radiative response, and remarkable resistance to radiation-induced degradation [3]. In particular, $CsPbI_3$ nanocrystals exhibit excellent scintillation properties, suitable for specific applications such as fiber-coupled real-time dosimetry**,** indeed they offer emission in the near infrared, which is critical to minimize spurious signals from intrinsic fluorescence of optical fibers, while maintaining high stability and luminescence efficiency under ionizing radiation. Optimizing $CsPbI_3$-based nanocomposites requires a detailed understanding of how structural and chemical properties influence carrier dynamics, including transport, trapping, and recombination processes, as these directly affect emission efficiency and timing. In this work, we investigate the luminescence behavior of $CsPbI_3$ nanocrystals, both dispersed in solution and embedded in polymer matrices, to evaluate the effects of environmental stabilization on their optical properties. The experimental study combines complementary spectroscopic techniques such as steady-state photoluminescence, radioluminescence, and time-resolved photoluminescence measured as a function of temperature to probe emission behavior, thermal effects, carrier lifetimes, and recombination dynamics. This approach enables the investigation of the interplay between trapping sites and luminescence dynamics in various environments, providing a comprehensive picture of carrier behavior in nanoscale perovskites. The results of this study provide fundamental insight into the mechanisms governing scintillation at the nanoscale and guidance for the rational design of $CsPbI_3$-based nanocomposite scintillators optimized for real-time dosimetry and advanced radiation detection applications, including emerging clinical techniques such as FLASH radiotherapy.

Keywords: Lead halide perovskite nanocrystals, scintillation, carrier dynamics.

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O-12. Diopside photocatalyst from agro-industry waste: Revolutionizing sustainable wastewater treatment

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Rapid industrial expansion has made water pollution to a key environmental threat. Factories frequently dump raw wastewater, loaded with heavy metals and dyes, directly into natural water sources without proper treatment. Wastewater must undergo treatment prior to environmental discharge. This paper details with an efficient sol-gel approach to produce diopside nanoparticles from agro-industry byproducts rice husk ash and ground granulated blast furnace slag. Analysis of XRD and FTIR data confirmed that the prepared powder is diopside, while FESEM revealed the morphologies of the synthesized material. The optical bandgap was determined from UV-visible absorption spectra using Tauc plots lies in the visible region, strongly enabling photocatalytic dye degradation via efficient electron-hole separation. Photocatalytic activity of the diopside nanoparticles was evaluated using methylene blue and methyl violet dyes. The impact of starting dye concentrations and catalyst amounts was examined on the visible-light-driven degradation efficiency of methylene blue and methyl violet dyes.

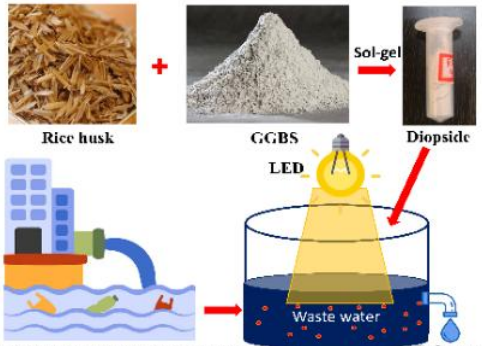

Fig1. Graphical abstract.

Keywords: diopside, methylene blue, methyl violet.

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O-13. Delithiation and temperature-induced behaviour in a Li_2MnO_3-$Li_{0.69}MnO_2$ core-shell system: A molecular dynamics study

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The structural degradation of Li rich layered cathodes such as O3-type Li_2MnO_3 remains a major obstacle to their practical application in high-energy lithium-ion batteries [1][2]. In this study, a core-shell architecture consisting of an O3-type Li_2MnO_3 core coated with an O2-type $Li_{0.69}MnO_2$ shell was investigated to evaluate its structural stability and lithium transport behaviour under varying thermochemical conditions. Molecular dynamics simulations were employed to examine the effects of delithiation from Li_2MnO_3 to Li_1MnO_3 and temperature variation on lattice stability and lithium diffusion within the core shell structure. Structural analysis revealed that the rigid O2 type shell constrains relaxation of the Li_2MnO_3 core, resulting in internal stress accumulation and lattice distortion at elevated temperatures (1500 K). Thermomechanical analysis further showed that while most lithium compositions maintain volumetric stability at moderate temperatures, pronounced volume expansion and surface area increases occur for $Li_{1.2}$ and $Li_{1.8}$ compositions above 1000 K, suggesting thermally induced structural transformations associated with oxygen activity and cation rearrangement. In contrast, intermediate compositions between $Li_{1.4}$ and $Li_{1.6}$ exhibit enhanced structural stability with minimal volumetric and surface fluctuations. Lithium diffusion analysis indicates increased ionic mobility at intermediate lithium concentrations and higher temperatures, highlighting the role of the O2 type shell in facilitating lithium transport while constraining structural relaxation. These findings provide important insights into the thermochemical and thermomechanical behaviour of Li rich core shell systems and offer guidance for the design of structurally stable cathode materials for next generation lithium-ion batteries.

Keywords: Delithiation, Core-shell, Lithium-ion batteries.

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O-14. Comparison of optical properties of Ga-doped ZnO thin films and NV rich single crystal diamond

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The nominally undoped ZnO thin films were pulsed laser deposited (PLD) on fused silica glass and used as a substrates for hydrothermally grown Ga-doped ZnO nanorods. Optical properties were measured using photothermal deflection spectroscopy (PDS) and frequency resolved photoluminescence spectroscopy (f-resolved PL). In our previous papers [Z. Remeš et al, J. Phys. Conf. Ser. 2712 (2024) 012004, Z. Remeš et al, J. Phys. Conf. Ser. 2931 (2024) 012011, and Z. Remeš et al, Phys._Scr. 100 (2025) 115910] we presented an upgrade of our spectrofluorometer optimize to measure the phase shift between sinusoidal UV excitation and PL emission at low temperature (4 K) using lock-in amplifier. Here we apply this method to evaluate the mean PL decay time of hydrothermally grown Ga-doped ZnO nanorods.

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O-15. Structural and Thermodynamic Stabilization of $Li_{1.2}Mn_{0.8}O_2$ Cathodes through Ti Doping: Insights from DFT and Cluster Expansion

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Lithium-rich and manganese-rich layered oxides offer high capacities and voltages, but their application is limited by poor cycling stability, voltage decay, and structural degradation. In this study, density functional theory (DFT) and cluster expansion methods were employed to investigate Ti-doped $Li_{1.2}Mn_{0.8}O_2$ and predict thermodynamically stable configurations. A composition with 10% Ti substitution was selected for detailed analysis to allow direct comparison with experimental data. The study evaluates structural properties, including lattice parameters and phase stability, thermodynamic behavior, and BET surface area, providing a comprehensive understanding of the material. The results reveal that Ti incorporation enhances structural robustness, stabilizes favorable phases, and optimizes surface characteristics, offering insights for the design of lithium-rich manganese-based cathodes with improved cycling performance and electrochemical stability.

Keywords: Lithium-ion batteries; $Li_{1.2}Mn_{0.8}O_2$, titanium doping

O-16. Interplay of optically- and magnetoactive energy levels of the Ce-doped $Y_3Al_5O_{12}$ nanopowders

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Ce-doped $Y_3Al_5O_{12}$ (YAG: Ce) nanopowders are widely studied luminescent materials, particularly used in biodetection to detect ionizing radiation. Composite systems incorporating luminescent nanocrystals significantly reduce the cost of detection technologies. The use of nanopowder has shifted the focus of YAG: Ce systems synthesis toward wet chemical methods. Consequently, a thorough investigation of the potential channels for energy transfer in nanocrystals is required, focusing on the interactions between Ce ions and their local environment within nanoscale YAG.

We report on the synthesis of nanoscale YAG: Ce (0.5, 1.5, 2, and 3 mol.%) crystals, which were synthesized by co-precipitating hydroxides from Y, Al, and Ce salts in an ammonia solution (pH = 9) and annealed at 1500°C for one hour. TEM and XRD analysis revealed that the 100-nm nanoparticles had a single-phase cubic YAG structure. The blue absorption and yellow emission of Ce^{3+}-doped YAG phosphors are attributed to the interconfiguration $4f^1 \leftrightarrow 4f^0 5d^1$ transitions of the Ce^{3+} ion. The participation of 5d energy levels makes these transitions sensitive to the site symmetry of the host lattice.

We analyzed the EPR spectra of the YAG: Ce samples using calculated angular dependencies in the (110) and (001) planes. The presence of at least two magneto-optical centers was revealed. The dominant component consists of Ce^{3+} ions that replace Y^{3+} ions in dodecahedral positions with D_2 site symmetry. These ions have six magnetically inequivalent positions and appear in EPR spectra as three doublets: J = ±1/2, ±3/2, and ±5/2. The smaller component consists of Ce^{3+} ions in octahedral positions, which are caused by Y_{Al} antisite defects. These ions manifest themselves in the EPR spectrum through a single doublet with M_J = 1/2. The large difference in the ionic radii of Ce^{3+} and Al^{3+} results in substantial distortion of the octahedral complexes. Additionally, we found that Ce^{3+} ions in dodecahedral positions can exhibit a ligand-hyperfine (LHF) structure due to the interaction between cerium's spin (S = ½) and the four ^{89}Y (I = ½) nuclei. Since the Y ions are at the same distance (≈ 3.7 Å), the expected intensity ratio is 1:4:6:4:1. However, distortions caused by the anisotropy of the Ce orbital state can complicate the LHF structure in [CeO_8] complexes. We also analyzed the possibility of an LHF structure arising from the interaction between Ce^{3+} and two ^{27}Al (I = 5/2) ions 3.00 Å apart, in which case the intensity ratios would be 1:2:3:4:5:6:5:4:3:2:1.

Acknowledgements: This research was partially supported by the DETMED project of the Horizon 2020 program.

Keywords: yttrium aluminum garnet, nanoscale powders, Ce^{3+} luminescence, EPR, ligand hyperfine structure

Poster presentations -abstracts-

P-01. Radiation-induced structural evolution of $NdGaO_3$ single crystals under 147 MeV krypton ion irradiation

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$NdGaO_3$ single crystals are of considerable interest due to their high radiation tolerance and potential applications in optoelectronics, radiation detectors, and functional oxide heterostructures. This study investigates radiation-induced structural modifications in $NdGaO_3$ crystals irradiated with 147 MeV krypton ions at fluences of 10^{11} and 10^{12} ions/cm^2.

X-ray diffraction (XRD) measurements performed in θ–2θ geometry reveal diffraction patterns dominated by (00l) reflections, indicating strong preferential orientation along the c-axis. The pristine crystal exhibits high structural quality with a lattice parameter c = 7.708 Å, consistent with literature values, and is characterized by sharp, symmetric peaks and low diffuse background.

Irradiation at 10^{11} ions/cm^2 results in a slight peak shift toward lower angles, corresponding to lattice expansion (c = 7.720 Å, $\Delta c/c \approx 1.6 \times 10^{-3}$). This behavior is attributed to the formation of irradiation-induced point defects, including vacancies and interstitials. Moderate peak broadening (FWHM: 0.10° → 0.16°) indicates the development of microstrain (~10^{-2}), while the overall crystalline order is largely preserved.

At 10^{12} ions/cm^2, structural degradation becomes pronounced due to ion track overlap and defect accumulation. The lattice parameter increases further to c = 7.744 Å ($\Delta c/c \approx 4.7 \times 10^{-3}$), accompanied by significant peak broadening (up to 0.30°), increased diffuse scattering, and reduced peak intensity. Peak asymmetry suggests the formation of a structurally heterogeneous, defect-rich near-surface layer.

The results indicate a transition from isolated point defect formation to a regime dominated by overlapping ion tracks and partial amorphization. The irradiated crystal can thus be described as a heterogeneous system consisting of a disordered surface layer and a relatively intact crystalline core.

These findings provide insight into radiation damage mechanisms in perovskite oxides under swift heavy ion irradiation. The observed structural stability at lower fluences and controlled defect evolution highlight the potential of $NdGaO_3$ as a robust substrate material for oxide electronics and heterostructures operating in harch radiation environments, including space and nuclear technologies.

Keywords: $NdGaO_3$, swift heavy ions, X-ray diffraction, radiation defects, lattice expansion, microstrain, ion tracks.

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P-02. Broadband luminescence of $NdGaO_3$ single crystals under high-energy excitation 45 eV

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$NdGaO_3$ single crystals are promising materials for applications in photonics, optoelectronics, and radiation detection due to their structural stability, optical transparency, and efficient rare-earth luminescence. This work presents a comprehensive study of the luminescence properties of $NdGaO_3$ under high-energy excitation (45 eV), provided by synchrotron radiation. For the first time, luminescence has been measured over an exceptionally broad spectral range spanning the ultraviolet, visible, and near-infrared regions (200–1060 nm), enabling a detailed analysis of radiative relaxation processes. Previous studies were restricted to measurements within the visible spectral range.

The excitation energy significantly exceeds the bandgap of the host lattice, resulting in the generation of high-energy electron–hole pairs and secondary electron cascades. Under these conditions, energy transfer from the host matrix to Nd^{3+} ions become highly efficient, and the emission spectrum is dominated by intra-center 4f–4f transitions of Nd^{3+}.

In the ultraviolet region (200–300 nm), a weak broad band is observed, attributed to high-energy matrix-related recombination and possible contributions from Nd^{3+} 5d states. In the 360–430 nm range, well-resolved narrow lines appear, corresponding to higher-energy 4f–4f transitions split by the low-symmetry crystal field of the orthorhombic perovskite structure.

The visible region exhibits distinct emission bands near 589 nm and 650–670 nm, associated with transitions from excited multiplets ($^4G/^2G$) to lower ^4I levels. In the ~800 nm region, multiple Stark components are observed, indicating intermediate relaxation pathways. The most intense emission is detected in the near-infrared range (865–930 nm), corresponding to the fundamental Nd^{3+} transition $^4F_{3/2} \rightarrow {}^4I_{9/2}$. This band displays a pronounced multi-peak structure due to Stark splitting, with a dominant peak near 877 nm. Additionally, the onset of the $^4F_{3/2} \rightarrow {}^4I_{11/2}$ transition is observed at 1.05–1.06 μm, although its maximum lies beyond the measured spectral range.

The results demonstrate that luminescence in $NdGaO_3$ under high-energy excitation is governed primarily by efficient energy transfer to Nd^{3+} centers, with minimal contribution from intrinsic matrix emission. These findings highlight the role of Nd^{3+} ions as effective luminescence centers and confirm the high structural quality of the investigated crystals, supporting their use in advanced photonic and radiation-detection applications.

Keywords: $NdGaO_3$, luminescence, VUV excitation, rare-earth ions, broadband spectroscopy, energy transfer.

References:

[1] S. Ghosh et.al. Scientific Reports 6, 36352 (2016).

P-03. Study of the kinetics of defect accumulation in the surface layers of high-entropy alloys under heavy ion irradiation

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This paper presents the results of an evaluation of the kinetics of point and cluster defect accumulation in the near-surface layer of high-entropy AlNbTiVZr alloys irradiated with high-energy heavy ions, simulating the effects of fission fragments. Interest in high-entropy alloys stems from their potential for use as structural materials for the first wall of high-temperature nuclear reactors exposed to high temperatures and high radiation doses. The studies established that, at low irradiation fluences, the accumulation of radiation damage is inhibited by the structural properties of high-entropy alloys, which inhibits the processes of destruction and diffusion of defects in the damaged layer. At fluences above 1012 ion/cm2, typical for areas of overlapping defect inclusions, cluster defects form. Their formation leads to an exponential change in the strength characteristics, causing the destruction and softening of the near-surface layer of the alloys. It was found that changing the irradiation temperature from 300 K to 500 K does not lead to serious differences in the structural changes and the degree of degradation of the alloys, while with an increase in the irradiation temperature to 700–1000 K, the degree of degradation of the damaged layer is more than two to three times higher than in the case of irradiation at a temperature of 300 K.

Keywords: radiation damage, high-entropy alloys, destruction of the surface layer.

P0-4. Sensitisation of OSL signals in quartz: Insights from multi-spectroscopic analysis of quartz from multiple geological settings

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Quartz optically stimulated luminescence (OSL) sensitivity and electron spin resonance (ESR) signals have been empirically proposed as indicators for sediment provenance. OSL sensitivity is defined as luminescence produced per unit dose (Gray: Gy) per unit mass (mg). The mechanisms driving OSL sensitization of quartz grain after detachment from source rocks remain an open question in the luminescence community. Most previous work has focused solely on sink sediments, while recent studies highlight the role of lattice defects in the source rocks in the OSL sensitisation process.

The present study investigates the OSL sensitization by dosing and bleaching of quartz from diverse rocks, including granites, sandstones, volcanic rocks, metamorphic rocks, and, in some cases, their derived sediments, with ages ranging from millions to billions of years. We combine thermoluminescence, OSL, ESR, cathodoluminescence (CL) and Raman spectroscopy, with geochemical data obtained through laser ablation inductively coupled plasma mass spectrometry (LA-ICPMS). Quartzes that showed OSL sensitisation following repeated cycles of laboratory dosing and bleaching exhibited the $[TiO_4\text{-}Li^+]^0$ electron centre in ESR, had notably high concentration of titanium and lithium impurities and had high blue emission in SEM-CL. Samples lacking these centres did not show any laboratory OSL sensitisation. We find a strong correlation of the degree of laboratory OSL sensitisation with the $[TiO_4\text{-}Li^+]^0$ electron centre and saturated $[AlO_4]^0$ hole centre from ESR signal, and the titanium and lithium concentrations measured by LA-ICPMS. Our data reinforce the idea that the potential for OSL sensitisation originates from specific lattice defect structures acquired by quartz during crystallisation.

Keywords: natural quartz, OSL sensitivity, ESR, CL, LA-ICPMS, titanium, lithium.

Acknowledgement: This research is funded by European Research Council ERC grant PROGRESS-CoG “Reading provenance from ubiquitous quartz: understanding the changes occurring in its lattice defects in its journey in time and space by physical methods”

P-05. Electron-beam dose dependence of the non-bridging oxygen hole centre in quartz across diverse rocks and sediments revealed by scanning electron microscopy: potential implications for provenance and thermochronology

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Despite being one of the stoichiometrically purest minerals (ideal formula SiO_2), quartz exhibits various intrinsic and impurity-related defects that contain important genetic information. We report scanning electron microscopy (SEM) coupled with cathodoluminescence (CL) wavelength-resolved spectroscopy on quartz from different rock types spanning a wide range of geological settings and ages to investigate defect phenomena. All samples show two main emissions: a red band at ~1.93 eV (~643 nm), attributable to non-bridging oxygen hole centres (NBOHC) defects, and a blue band at ~2.7 eV (~450 nm), explained by Ti-related defects. The origin of NBOHCs is relatively well understood and may result from intrinsic mechanisms or extrinsic pathways involving radiolysis of passivated precursor sites such as hydroxyl-related defects. Radiation-damage experiments under controlled electron irradiation in SEM provide a tool to study defect formation dynamics. We investigate the evolution of the NBOHC defect at different irradiation times (electron doses). CL acquired during SEM irradiation shows monotonic growth of the ~1.9 eV emission described by the sum of two saturating exponentials, interpreted as coexistence of hydroxyl-mediated defect generation and intrinsic rupture of Si–O–Si bridges or peroxy Si–O–O–Si linkages. SEM-induced NBOHC luminescence is therefore controlled by the balance between hydrogen chemistry and intrinsic bond rupture, reflecting quartz geological type. The initial CL intensity records the natural balance among α-radiation damage, thermal resetting, and hydrogen passivation. These relations suggest CL from the NBOHC as a potential quartz-intrinsic provenance indicator or thermochronometer.

Keywords: quartz; cathodoluminescence; non-bridging oxygen hole centre (NBOHC)

Acknowledgement: This research is funded by European Research Council ERC grant PROGRESS-CoG “Reading provenance from ubiquitous quartz: understanding the changes occurring in its lattice defects in its journey in time and space by physical methods”

P-06. Up-conversion luminescence and multimodal temperature sensing behaviors in the visible and infrared region of Er^{3+} and (Er^{3+}, Yb^{3+}) ions in $Ca_3Ta_2Ga_3O_{12}$ phosphors

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The CTGG ceramic samples, single-doped with Er^{3+} ions and co-doped with (Er^{3+}, Yb^{3+}) ions, were obtained by the solid-state reaction method and the optimal concentrations of Er^{3+} and (Er^{3+}, Yb^{3+}) ions in terms of emission intensity in the visible domain were determined. Green and red up-conversion (UC) emissions under 973 nm and 1550 nm excitations via $Yb^{3+}\rightarrow Er^{3+}$ cooperative energy transfer processes were obtained. The dependence of green and red UC luminescence intensities as a function of the excitation density power at 973 nm has been characterized. The decay time of the $^4S_{3/2}$ level of Er^{3+} ions was measured in all samples, and the efficiency of the $Yb^{3+}\rightarrow Er^{3+}$ energy transfer was discussed. Two methods were used here, Luminescence Intensity Ratio (LIR) for different thermally coupled (TCLs) and thermally coupled (NTCLs) levels, and fluorescence lifetime (FL). Thus, the emission spectra of Er^{3+} ions were measured at different temperatures in the range of 150–575 K and excitation wavelengths of 973 nm and 1550 nm. Multimodal temperature sensing behaviors of LIR were focused on TCLs ($^2H_{11/2}$/$^4S_{3/2}$), NTCLs ($^2H_{11/2}$/$^4F_{9/2}$), and infrared TCLs ($^4I_{13/2}$ (1,2,3)). The FL method was applied for the emission kinetics of the $^4S_{3/2}$ level of Er^{3+} ions.

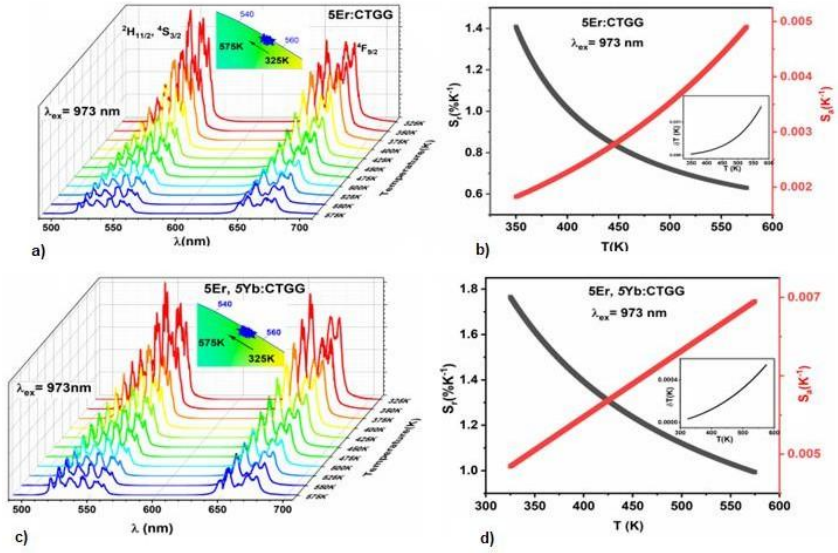

Fig. 1 Temperature dependence emission spectra of 5Er: CTGG (a) and 5Er, 5Yb: CTGG (c) under 973 nm excitation and their CIE chromaticity diagram as insets. The S_r and S_a curves (b, d).

Keywords: Up-conversion, Spectroscopy, Sensors.

Acknowledgements: This work was supported by the Romanian Ministry of Education and Research, under the National Nucleu Program LAPLAS VII - contract no. 30N/2023 and CCCDI - UEFISCDI, project number PN-IV- P6-6.1-CoEx2024-0154, within PNCDI IV.

P-07. Photochromism and photorefraction in (Bi,Mg)-codoped stoichiometric $LiNbO_3$ governed by lone pairs and exciton-polaronic processes

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Recently outstanding results on photorefractive holography in (Bi,Mg)-codoped congruent lithium niobate (LN) have been reported [1]. As the photochromic effect often degrades the quality of photorefractive devices, an investigation of the long-term dynamics and mechanism of photochromism in (Bi,Mg)-codoped stoichiometric LN has been carried out [2]. In the present work this is extended to the ms to min time range, also applying two-wave mixing experiments allowing to separate photochromic and photorefractive effects.

Czochralski-grown samples with a Li/Nb ratio of 1.38:1, Bi concentrations of 2 or 4 mol%, and Mg concentrations of 1 or 2 mol% (all data in the melt) were used to investigate both photochromic and photorefratctive effects using 405 and 443 nm lasers in the temperature range between 10 and 45°C. A two-wave mixing simulator program was developed based on a one-center model involving photochromic and various photorefracive mechanisms.

Apart from the persistent light-induced absorption reported earlier and small transients on the ms timescale, one or more important photochromic component(s) were found to be saturating on a subsecond and decaying on a subminute timescale, the recovery governed by an activation energy of ~0.6 eV. Photorefractive response was slightly faster with $\tau \approx 30$ ms. The ratio of the photorefractive and photochromic diffraction efficiencies was determined as a function of the input intensity showing the domination of the photorefractive one for total input intensities above some tens of mW/cm^2. Estimates of the recombination coefficient and the effective cross section for electron excitation by photon absorption could also be derived.

The effects for low intensities are discussed in terms of localized exciton-polaronic effects next to the lone pairs on various Bi^{3+}-defect complexes also including the Mg-codopant. While these may explain the various time ranges in photochromism, exciton dissociation with increasing laser intensity also provides the liberated polarons responsible for photodiffraction on a similar time scale. The obtained excitation and activation energies lead to a model of metastable gap states with various lifetimes. The results are helpful for optimizing holographic systems and underline the importance of excitonic scenarios in LN [3] in general.

Keywords: $LiNbO_3$, self-trapped excitons, photochromism/photorefraction,.

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P-08. Multilevel modelling applied to $KMgF_3$: a hybrid classical-quantum mechanical approach

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A multilevel modelling approach was applied to $KMgF_3$ and aimed at the study of its structural, electronic, and optical properties with reduced computational cost. The strategy employs a two-step procedure where classical atomistic modelling is responsible for structural optimisation, defect screening, defect formation energetics and relaxation based on empirical potentials, while the quantum step performs electronic calculations using the atomic positions previously obtained. For classical modelling, the GULP code was used, while quantum modelling employed DFT with GGA functional and ultrasoft pseudopotentials inside the Quantum ESPRESSO package. The multilevel strategy reduced by up to 99.8% the structural optimisation time and by approximately 56.8% the computational cost of calculating electronic and optical properties. For the perfect $KMgF_3$ lattice, an indirect energy gap (R→Γ) was identified, with the valence band maximum dominated by F 2p orbitals and the conduction band arising from partial hybridisation of K 3p/4s orbitals, with a smaller contribution from Mg 3s states. The optical absorption spectra showed an increase starting at 7 eV with a bump close to 8 eV followed by a steep increase around 10.5 eV which is typical of indirect band gap materials. In the analysis of intrinsic defects, the pseudo-Schottky KF defect was found to be energetically most favourable. Modelling of the 3×3×3 defective supercell revealed an isolated and almost flat band around 7.0 eV, indicating a high effective mass and low carrier mobility, thus characterising a trapping state. These results confirm the robustness and scalability of this multilevel approach for the efficient study of defects in materials.

Keywords: Multilevel modelling; $KMgF_3$; DFT; Atomistic simulation; Defects

P-09. Energy transfer in the (Pr, Yb): $Ca_3(Nb, Ga)_5O_{12}$ phosphor with excellent properties for temperature sensing applications

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Pr^{3+} and Yb^{3+} co-doped $Ca_3(Nb, Ga)_5O_{12}$ - (Pr, Yb): CNGG ceramic phosphors were sintered using the solid-state reaction method. The luminescence of Pr^{3+} and Yb^{3+} ions resulting from different optical processes, such as down-conversion (DC) and up-conversion (UC), was highlighted in the (Pr, Yb): CNGG phosphors. Under blue (457 nm) and near-infrared (973 nm) excitation, co-doped phosphors emit visible light through DC and UC processes caused by different *f-f* transitions of Pr^{3+} ions. These processes exhibit high energy transfer efficiencies of η_{DC} = 65 % and η_{CET} = 73%, respectively. The temperature dependence of Pr^{3+} ion luminescence was characterized based on the luminescence intensity ratio (LIR) within the temperature range of 10-500 K (Fig. 1). Due to the efficient energy transfer from Yb^{3+} to Pr^{3+}, the highest values of relative thermal sensitivity (S_r) (Fig. 2) were found to be 5.9 % K^{-1} at 175 K for the (1Pr, 4Yb) sample and 6.9 % K^{-1} at 10 K for the (10Yb, 2Pr) sample. This indicates that (Pr, Yb): CNGG phosphor is a promising candidate for cryogenic optical temperature sensing.

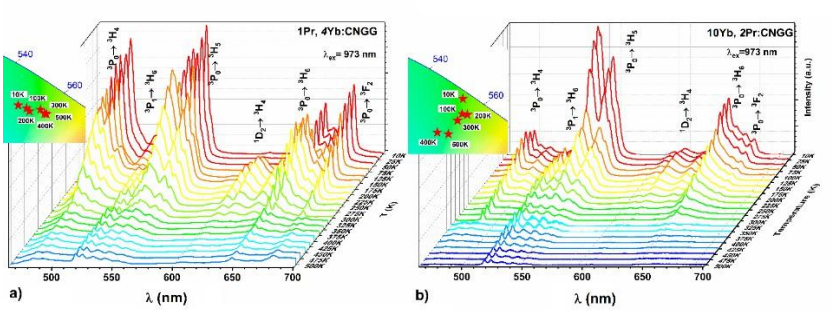

Fig. 1. Temperature dependence of Pr^{3+} emission spectra in (1Pr, 4Yb) (a) and (10Yb, 2Pr) (b) samples and their CIE chromatic diagram as insets

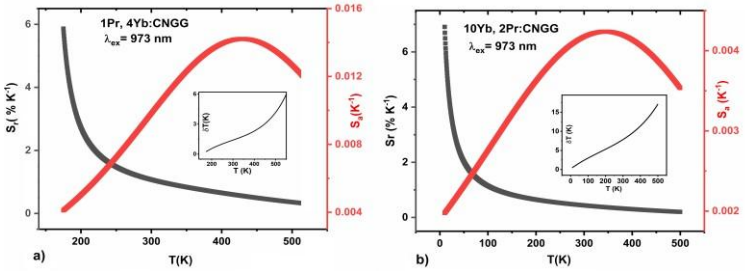

Fig. 2. The S_r and S_a curves, together with temperature uncertainty δT as insets, for (1Pr, 4Yb) and (10Yb, 2Pr) (b) samples

Keywords: Phosphor, (Pr^{3+}, Yb^{3+}), Up/down-conversion photoluminescence, temperature sensing

Acknowledgments: This work was supported by the Romanian Ministry of Education and Research, under the National Nucleu Program LAPLAS VII - contract no. 30N/2023 and CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0154, within PNCDI IV. We also thank the INFLPR

P-10. Radiophotoluminescence response of color centers in lithium fluoride thin films for gamma-ray dosimetry

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Passive solid-state detectors based on 2 µm-thick lithium fluoride (LiF) thin films, grown by thermal evaporation on different substrates (Suprasil®, Si(100) and aluminum deposited on silicon) at ENEA C.R. Frascati, were irradiated at six doses in the range from 10 to 10^3 Gy, at three dose-rates along the entire dose range, with the ^{60}Co source of the Calliope irradiation facility at ENEA C.R. Casaccia [2]. These radiation detectors exhibit high intrinsic spatial resolution over a large field of view, a wide dynamic range and ease of use, as they are insensitive to ambient light and do not require chemical development. Their operating principle is based on the optical readout of the visible radiophotoluminescence (RPL) emitted by radiation-induced F_2 and F_3^+ color centers (CCs) [1]. After irradiation, the RPL of the LiF films was measured by a Nikon Eclipse 80i fluorescence microscope equipped with an Andor NEO sCMOS camera and a blue LED source. The integrated RPL signal intensity due to F_2 and F_3^+ CCs showed a linear behavior as a function of the irradiation dose over the investigated dose range, independently from the dose-rate. Due to high stability of the CCs at room temperature, the RPL measurements can be repeated without signal fading. Furthermore, the detectors can be reused after erasing of the CCs through thermal annealing. These results demonstrate the potential of LiF film-based detectors for gamma-ray dosimetry over a very wide dose range.

Keywords: lithium fluoride, thin films, gamma rays.

References:

[1] J. Nahum, Phys. Rev. **158**, 814 (1967).

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Acknowledgments

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P-11. AI/DFT modeling of Mn-doped $BiVO_4$ photocatalyst

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$BiVO_4$ is one of the most promising visible-light-responsive photoanodes for hydrogen production from water splitting because of its suitable band gap, chemical stability, and low cost [1]. However, its practical photoelectrochemical efficiency remains limited by relatively poor charge-carrier mobility and rapid electron-hole recombination. In this computational study, we combine DFT calculations and AI-assisted analysis to investigate Mn-doped $BiVO_4$ as a tunable photocatalyst for visible-light-driven applications.

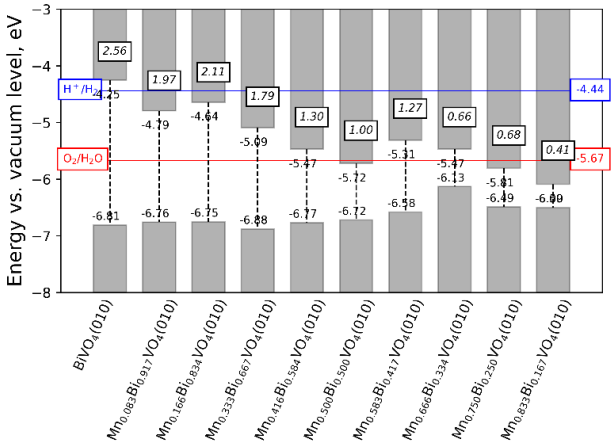

Fig.1. Calculated band-edge positions of Mn-doped $BiVO_4$.

Obtained results show that Mn doping systematically alters the VB and CB positions of $BiVO_4$ that leads to narrowing of the band gap of undoped $BiVO_4$ (Fig.1). This electronic structure tuning can extend light absorption further into the visible region while preserving energetically favorable redox characteristics for photocatalytic reactions. AI and machine-learning analysis of DFT-derived descriptors further indicate that Mn concentration is one of the key variables governing the predicted performance of the material. These results provide a rational basis for identifying promising doping windows without relying exclusively on costly trial-and-error calculations or synthesis.

Keywords: water splitting, $BiVO_4$, doping, photocatalytic reactions

References:

[1] J. Su, L. Guo, N. Bao, C. A. Grimes, *Nano Lett.*, **11**, 1928-1933 (2011).
[3] S. Balu, S.-W. Chen, S. Piskunov, et al., *Adv. Compos. Hybrid Mater*, **7** (2024) 32.

P-12. EPR of neutron-radiation-induced defects in $Gd_3Ga_5O_{12}$

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When GGG is irradiated with threshold neutron (E = 0.1 eV) beam at a fluence of 10^{20} cm^{-2} along the [111] crystallographic axis, several new paramagnetic defects emerge. The most prominent among them is a germanium (Ge) impurity, formed via neutron capture by gallium (Ga). By combining literature data [1] with density functional theory (DFT) calculations, this defect is proposed to exist in the $4s^2 4p^1$ (Ge^+) charge state. For such a center to stabilize in GGG, multiple oxygen vacancies must be present to compensate for charge imbalance. Additionally, the observed EPR signals lack the angular dependence typical of cubic symmetry, suggesting that significant structural distortions occur due to neutron irradiation [2].

Other detected defects are tentatively attributed to rare-earth ion impurities, though their exact identification remains elusive due to temperature-dependent resonance shifts. These variations may indicate a magnetic phase transition influencing the EPR signal behavior in irradiated GGG [3].

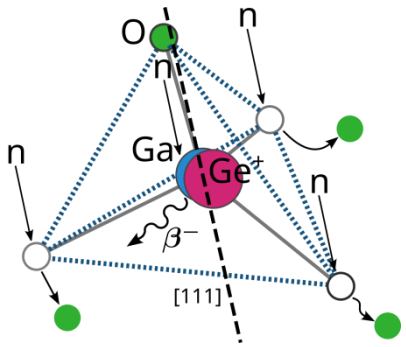

Figure 1: *Ge^+ with 3 O^{2-} vacancies substituting Ga in tetrahedral site.*

Keywords: neutron-radiation-induced defects, electron spin resonance (ESR), gadolinium gallium garnet

References:

[1] N. Mironova-Ulmane et. al., *Nucl. Instrum. Methods Phys. Res. B* **480**, 22 **(2020)**
[2] J. Cirulis et. al., Radiat. *Phys. Chem*., 113664 **(2026)**
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Acknowledgements: This work was supported by the European Regional Development Fund and Latvian state budget grant in the framework of the project [No. 1.1.1.8/1/24/I/003].

P-13. Pr^{3+} doped $Ca_3(Ta,Ga)_5O_{12}$ single crystal

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Structurally disordered Pr^{3+}-doped $Ca_3(Ta,Ga)_5O_{12}$ - Pr:CTGG single crystal was grown by the Czochralski technique [1] and its spectroscopic properties were investigated. Modified Judd-Ofelt analysis was applied to determine the spectroscopic and laser emission characteristics. Based on the absorption and emission spectra at low temperature, the partial energy levels of Pr^{3+} ions have been obtained and a multicenter structure of the optical spectra was highlighted. The electron-phonon interactions were also observed in the emission spectra corresponding to the $^3P_0 \rightarrow {}^3H_4$ transition under different excitation wavelengths. The fluorescence decays of the $^3P_0$ and $^1D_2$ levels were measured. The emission cross-sections corresponding to the $^3P_0 \rightarrow {}^3H_4$ and $^3P_0 \rightarrow {}^3F_2$ transitions, quantum efficiency, gain bandwidth, and optical gain were determined. The obtained results indicate that the Pr:CTGG crystal has a high potential for obtaining efficient laser emission in the blue and red domains.

Figure 1*: As-grown Pr:CTGG single crystal. The inset shows a polished crystal sample cut from the grown crystal.*

Keywords: Czochralski, praseodymium, laser crystal.

References:

[1] C. Gheorghe, S. Hau, L. Gheorghe, A. Broasca, M. Greculeasa, F. Voicu, G. Stanciu, M. Enculescu, *Opt. Mater.* **150** 115286 (2024).

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P-14. Trefoil defects as a tuning mechanism for electronic and optical properties of molybdenum dichalcogenides

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Defect engineering provides an efficient route for tuning the properties of two-dimensional TMDs [1]. In this work, we investigate the effect of trefoil-type defects on the electronic structure and optical absorption of MoS_2 and $MoSe_2$ using DFT. The calculations are performed using two complementary approaches: the SOGGA XC-functional and the DFT+U method with on-site Coulomb corrections. Atomic models of defective structures and corresponding optical spectra are analyzed in comparison with pristine systems. The introduction of trefoil defects leads to the formation of localized electronic states within the bandgap, predominantly originating from Mo-*d* and chalcogen-*p* orbitals. The DFT+U approach captures the enhanced localization of defect states and improves the description of electronic correlations, while SOGGA provides a consistent description of the electronic structure and optical response. Both approaches reveal significant modification of the density of states near the Fermi level and bandgap narrowing in the presence of defects. The optical absorption spectra exhibit pronounced changes, including the emergence of additional low-energy peaks in the sub-bandgap region and redistribution of spectral weight. A comparative analysis between pristine and defected MoS_2 and $MoSe_2$ demonstrates that trefoil defects play a crucial role in enhancing infrared absorption and tailoring the optical response [2].

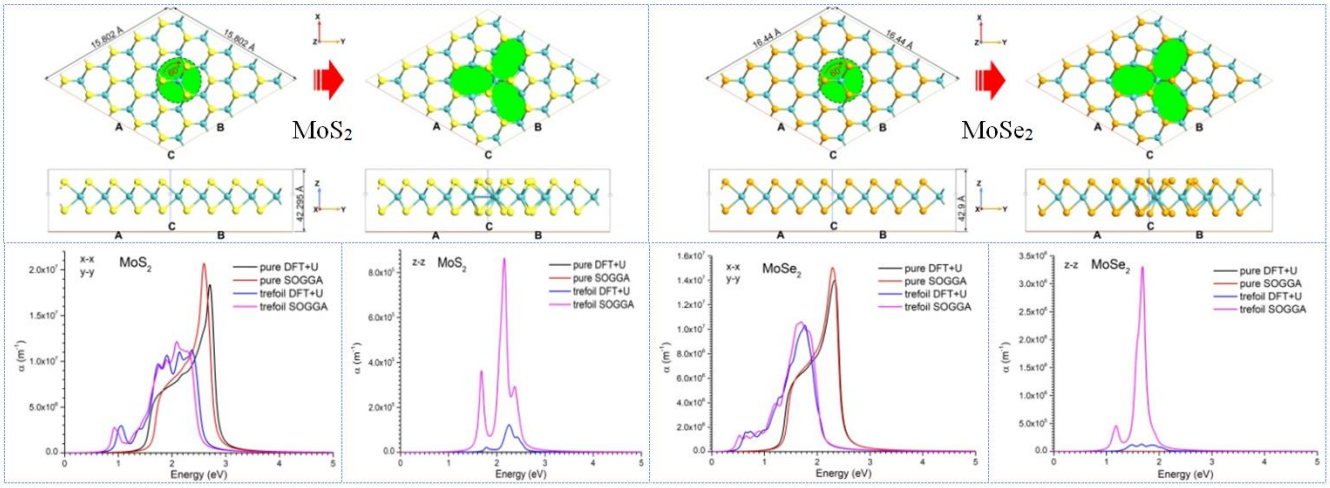

Figure 1: *Atomic structure of trefoil defects and corresponding optical absorption spectra of MoS_2 and $MoSe_2$*

Trefoil defects effectively tune the optoelectronic properties of molybdenum dichalcogenides for nanoscale optoelectronic and sensing applications.

Keywords: Trefoil defects; Molybdenum dichalcogenides; Optical absorption.

References:

[1] S. Manzeli et al., *Nature Reviews Materials* **2**, 17033 (2017).
[2] Q. Liang et al., *ACS Nano* **15**, 2165 (2021).

P-15. Dislocations in TbF_3 doped CaF_2 crystals

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Tb^{3+}-doped CaF_2 single crystals are attractive materials for green photonic applications. On the other hands, CaF_2 host shows low phonon energy and high optical transparency in the UV-VIS-NIR spectral region [1]. However, imperfections in the crystal structure can affect laser performance. Therefore, investigating dislocations is essential, as the density of dislocations serves as an indicator of the crystal's overall quality.

Three concentrations of TbF_3 -doped CaF_2 crystals have been grown using vertical Bridgman–Stockbarger method under high vacuum conditions (10^{-1} Pa) in a pure graphite crucible [2].

In this work, we examine the morphology of etch pits and the dislocation density using the chemical etching method [3]. This technique involves immersing a cleaved sample in 4N HCl at 60 °C for 5 minutes. During the process, small pits form at the points where dislocations emerge at the surface. These etch pits exhibit irregular hexagonal shapes. The dislocation density varies depending on the concentration of Tb^{3+} ions.

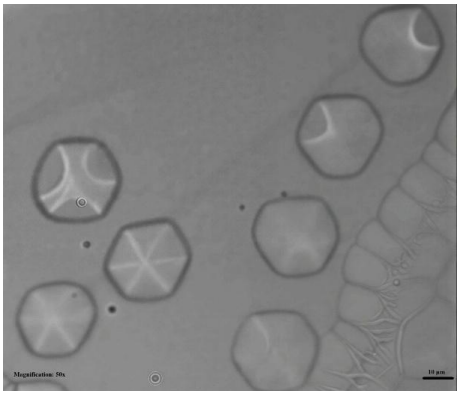

Figure 1: *Dislocations in CaF_2 crystal doped with 1 mol% TbF_3 - magnification 50X.*

Keywords: Calcium fluoride crystals, Defects, Dislocations.

References:

[1] Boubekri, H.; Diaf, M.; Labbaci, K.; Guerbous, L.; Duvaut, T.; Jouart, J.P. Synthesis and optical properties of Tb^{3+} doped CdF_2 single crystals. *J. Alloys Compd.* **575,** 339–343 (2013).

[2] D. Nicoara and I. Nicoara, *Mater. Sci. Eng. A* **102** L1 (1988).

[3] S. Amelinckx, The direct observation of dislocations, *Academic Press*, N.Y., (1964).

Acknowledgements: This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0154, within PNCDI IV

P-16. Host lattice influence on the visible emission of Tm^{3+} in CaF_2 and BaF_2 crystals

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Fluoride crystals doped with rare-earth ions have been widely investigated due to their favorable spectroscopic properties and low phonon energies, which reduce non-radiative relaxation processes and enhance luminescence efficiency. Among them, thulium-doped fluorides are considered promising materials for visible and infrared photonic applications. In this work, we comparatively investigate the visible emission properties of Tm^{3+} ions in CaF_2 and BaF_2 crystals grown by the vertical Bridgman method.

Optical absorption and photoluminescence measurements were performed in the UV-VIS spectral region for several TmF_3 concentrations. In CaF_2:Tm^{3+} crystals, UV excitation gives rise to several emission bands associated with radiative transitions of Tm^{3+} ions, particularly around 358, 449, 482, 510 and 690 nm. The emission intensity strongly depends on the dopant concentration, showing concentration quenching at higher TmF_3 contents.

In BaF_2:Tm^{3+} crystals, the emission spectra are dominated by intense violet and blue bands centered near 363 nm ($^1D_2 \rightarrow {}^3H_6$) and 450 nm ($^1D_2 \rightarrow {}^3F_4$). The strong blue emission and the measured lifetime of the 450 nm band highlight the potential of BaF_2:Tm^{3+} crystals for visible photonic applications. The concentration dependence of the emission intensity suggests a transition from isolated-ion behavior to interaction-dominated regimes at higher dopant concentrations.

Comparative analysis shows that the host lattice significantly influences the spectral distribution and emission efficiency of Tm^{3+} ions. Differences in crystal-field symmetry, local structure and phonon energy between CaF_2 and BaF_2 modify the radiative transition probabilities and the relative intensities of visible emission bands.

Keywords: fluoride crystals, thulium ions, photoluminescence, visible emission, rare-earth doped materials

References:

[1] C. Schornig, M. Ștef, G. Bușe, M. Poienar, P. Veber, D. Vizman, *Materials* 17, 4965 (2024)

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Acknowledgements: This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0154, within PNCDI IV

P-17. Activation of the dosimetric properties of alkali metal chlorides by light lithium and sodium ions

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Crystals of LiF doped with cationic impurities (LiF:Mg,Ti and LiF:Mg,Cu,P) are commonly used as dosimetric materials in detectors such as TLD-100 and TLD-700H, enabling the measurement of ionizing radiation doses up to approximately 10 Gy. In these systems, the principal dosimetric features correspond to high-temperature peaks of thermally stimulated luminescence (TSL) at 473 K for TLD-100 and 490 K for TLD-700H

A systematic investigation [1–3] was carried out into the dosimetric characteristics of alkali metal chlorides activated by light isovalent cations of lithium and sodium (NaCl:Li, KCl:Li, KCl:Na and RbCl:Na). Studies involved the registration and analysis of high-temperature TSL peaks, TSL spectra, tunnel luminescence (TL), the TL kinetics, and optical absorption associated with the concentration of radiation-induced defects in order to elucidate a common mechanism for the enhancement of the dosimetric peaks' light yield.

The experiments revealed pronounced dosimetric TSL peaks at 530 K for NaCl:Li, 505 K for KCl:Li, 570 K for KCl:Na, and 550 K for RbCl:Na. Their spectral composition was characterized by emission maxima at 3.4 eV for NaCl:Li, 2.8 eV and 3.1 eV for KCl:Li and KCl:Na, and 3.48 eV for RbCl:Na. For all investigated crystals, the X-ray luminescence (XRL) spectra coincide with the TSL and TL spectra, providing the basis for interpreting the nature of the observed TSL peaks. A principal effect has been identified: (i) Upon exposure to ionizing radiation, lithium (sodium) ions enhance the efficiency of the formation of halogen molecular centers (V_2, V_{2A}, V_3-centers), thereby creating energetically favorable conditions for the dominant mechanism of radiation defect formation - the association of interstitial halogen atoms; (ii) During thermal destruction of intrinsic radiation defects (V_2, V_{2A}, V_3- and *F*-centers), lithium (sodium) ions facilitate, within their local field, the recombination of free electrons with non-relaxed holes, leading to the formation of exciton-like luminescence centers.

These results suggest that a closely related mechanism may govern the operation of thermoluminescent dosimeters of the TLD series currently employed in radiation dosimetry.

The research work has been funded by Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP23488688).

Keywords: alkali halide crystals, thermally stimulated luminescence (TSL), dosimetric TSL peaks, tunnel luminescence (TL), X-ray luminescence (XRL), radiation defects.

References:

[1] K. Shunkeyev, A. Kenzhebayeva, A. Krasnikov, et al., *Optical Materials: X* **25**, 100395 (2025).
[2] K. Shunkeyev, A. Kenzhebayeva, Sh. Sagimbayeva, et al., *Journal of Luminescence* **284**, 121308 (2025).
[3] K. Shunkeyev, A. Kenzhebayeva, Sh. Sagimbayeva, Z. Serikkaliyeva, *Crystals* **15**, 67 (2025).

P-18. Luminescence enhancement via purposeful doping of alkali halide crystals by lithium and sodium ions

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The radiative decay of different electronic excitations formed in NaCl:Li, KCl:Li, KCl:Na, and RbCl:Na single crystals under the excitation by X-rays (W, 3 mA, 100 keV) or photons in vacuum ultraviolet (VUV) spectral region (using synchrotron radiation facility ad DESY, beamline P66) have been investigated in a wide temperature region.

Intense X-ray luminescence bands peaked around 3.4 eV in NaCl:Li, 2.8 eV and 3.1 eV in KCl:Li and KCl:Na, as well as at 3.4 eV in RbCl:Na have been detected (see also [1]). The enhancement of these emission bands follows the rise of lithium concentration (up to 400 ppm) as well as the crystal heating from 85 to 400 K. Based on the correlated increase with temperature of both the luminescence band intensity ($I \sim f(T)$) and the value of mean free path for non-relaxed holes ($\sigma(h) \sim f(T)$) prior their self-trapping, it has been suggested that just the introduction of Na^+ and Li^+ impurity ions facilitates the temperature-stimulated creation of exciton-like formations (bound excitons) in the process of electron-hole recombination nearby an impurity ion.

VUV photons of 7.6 eV directly generate free exciton-like formations in KCl:Li and KCl:Na crystals at 4.2 K. The following relaxation of electronic excitations results in the arisen photoluminescence band at 2.8 eV, which has been ascribed to the excitons localized in the field of lithium and sodium impurity ions – $e_S^0(Li^+)$ and $e_S^0(Na^+)$, respectively. In contrast to the case of X-ray excitation, these 2.8-eV photoluminescence bands undergo quenching with temperature rise and practically disappear to 200 K.

The excitation of KCl:Li and KCl:Na crystals by photons of $h\nu$ = 11-12 eV, the energy of which surely exceeds the formation energy of one-halide (free) anion excitons (about 8 eV) and the bandgap value (E_g = 8.8 eV), cause the appearance of intense luminescence bands at 2.8 eV and 3.1 eV, i.e., similar to those observed in these crystals under X-ray excitation and ascribed to recombinationally formed exciton-like formations in the field of light-weight impurity ions (Li^+, Na^+). The formation mechanisms and detailed origin of these bound excitons, decaying with luminescence even at 300-400 K, have been considered.

The study has been funded by Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP23488688).

Keywords: exciton-like formations, X-ray and photoluminescence, alkali halides.

References:

[1] K. Shunkeyev, A. Kenzhebayeva, et al., *Optical Materials: X* **25**, 100395 (2025).

P-19. Technology of the dosimetric alkali halide crystals growth in an argon atmosphere based on the Bridgman method

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The purification and growth of alkali halide crystals have been demonstrated using the KCl:Li crystal as an example on a universal crystal growth facility (Across International, USA). The technological procedure includes several sequential stages: (i) a deep static vacuum (10^{-3} Pa or 10^{-6} Torr) is created within a quartz reactor containing a quartz ampoule with the charge; (ii) high-purity argon is introduced at room temperature to 0.3–0.5 bar, selected so that, upon reaching the melt temperature (770–830°C), the internal pressure increases to approximately 1.1–1.3 bar – a measure for suppressing the aggressive vapors.

A wide range of thermal regimes, controlled by the Eurotherm 3204 multisegment controllers, provides considerable flexibility in designing temperature programs for both pure and doped crystals using 2 or 3-zone configurations. Of particular importance is the capability, implemented for the first time, of controlled slow-cooling stage of the grown crystal at a rate of 20–30°C/h. The mechanical translation of the quartz ampoule containing the charge is controlled through a SCADA system (Supervisory Control and Data Acquisition) operating within the MCGS environment (Monitor and Control Generated System), which functions as a human–machine interface (HMI) platform.

The proposed integrated crystal growth system differs significantly from conventional designs and eliminates several technological requirements: (i) quartz laboratories for sealing ampoules, since the raw material remains under vacuum within the quartz reactor itself; (ii) supplementary water cooling of the installation, because the crystallization center is maintained by the thermal block, while the ends of the quartz tube are positioned outside the hot zone. To further suppress halogen vapors, a special quartz shielding cover has been developed: two nested quartz cups that create a labyrinth-type barrier for the vapors.

In test measurements, X-ray luminescence (XRL) spectra of freshly grown KCl:Li crystals were recorded as a function of lithium ion concentration. The experiments revealed the expected enhancement of the luminescence light yield, which can be attributed to the recombination assembly of electron–hole pairs in the field of lithium ions. This effect represents an important parameter for the development of the scientific basis of scintillation detectors.

The research work has been funded by Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP26100001).

Keywords: alkali halide crystals, crystal growth, Bridgman method, X-ray luminescence (XRL).

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P-20. DFT Study of polysulfobetaine–hydronium interactions for PEM applications

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Proton exchange membrane (PEM) fuel cells are promising clean energy technologies, yet their widespread adoption remains limited by membrane materials that suffer from inadequate proton conductivity under low humidity and insufficient chemical stability during operation. This study investigates the atomistic interactions between hydronium ions (H_3O^+) and polysulfobetaine (PSB)—a zwitterionic polymer with covalently bonded cationic and anionic groups—to evaluate its potential as a next-generation PEM material. Density functional theory (DFT) calculations at the B3LYP/6-311++G(d,p) level were performed on a PSB monomer complexed with H_3O^+ in an explicit water environment. Geometry optimizations revealed preferential binding configurations, while Mulliken charge analysis quantified charge redistribution upon complexation. Bond length variations, molecular electrostatic potential (MEP) mapping, and frontier molecular orbital (HOMO-LUMO) analysis provided comprehensive insights into the electronic structure and reactivity changes [1].

Hydronium ions bind strongly and selectively to the sulfonate group (SO_3^-) of PSB through directional hydrogen bonds, inducing significant conformational changes in the polymer side chain. Charge transfer from sulfonate to hydronium weakens the O–H bonds of H_3O^+, reducing the energy barrier for proton dissociation. The HOMO-LUMO energy gap narrows upon complexation, indicating enhanced chemical reactivity and polarization. MEP maps confirm electrostatic complementarity between the negatively charged sulfonate and positively charged hydronium, while also showing modulated potential that prevents excessive proton trapping. Polysulfobetaine demonstrates an ideal balance of strong hydronium coordination and facilitated proton release—essential requirements for efficient Grotthuss-type proton transport. These atomistic insights provide a rational foundation for designing PSB-based PEMs with improved conductivity under diverse hydration conditions, advancing the development of durable, high-performance fuel cell membranes [2].

Keywords: Polysulfobetaine, hydronium ion, proton exchange membrane, density functional theory, proton transport mechanism

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P-21. Unveiling the Electronic and Vibrational Signatures of Radiation Defects in Cubic ZrO_2: A Synergistic DFT and Machine Learning Approach

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Radiation-induced defects critically influence the structural stability and functional performance of zirconia in nuclear and photocatalytic environments. A detailed atomistic understanding of vacancy formation, migration, and defect-induced electronic states remains challenging using conventional approaches alone. Integrating Density Functional Theory (DFT) with Machine Learning (ML) enables accurate, scalable modeling to bridge this gap and predict defect behavior across relevant time and length scales. In this study, we employ a combined DFT) and ML modeling framework to investigate radiation-induced defects in cubic zirconia (ZrO_2), with a specific focus on vacancies, *F*, and *F*+ centers (oxygen vacancies with 2- or 1-trapped electrons). The DFT method is used to accurately compute defect formation energies, migration barriers, and changes in electronic structure, while ML trained on DFT data facilitate large-scale simulations to capture defect migration and clustering over extended time scales relevant for photocatalytic applications. Our findings reveal that oxygen vacancies and associated F/F^+ centers introduce localized states within the bandgap, significantly altering the electronic properties and giving rise to defect-induced optical absorption features.

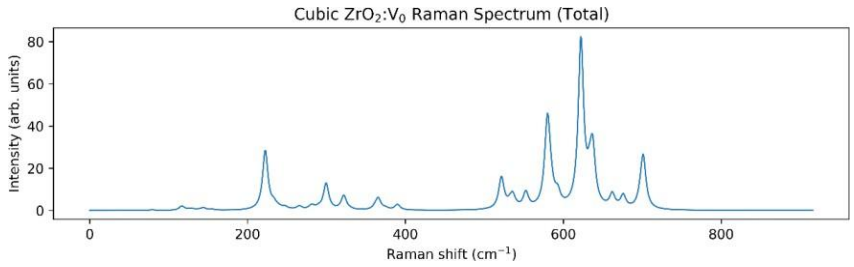

Figure 1: Calculated Raman spectra of vacancy containing cubic ZrO_2.

Raman spectroscopy simulations indicate that these defects lead to characteristic shifts and intensity variations in the vibrational spectra (Fig.1), correlating well with experimental observations. The results demonstrate that the integration of *ab initio* calculations with ML techniques not only enhances computational efficiency but also provides comprehensive microstructural insights into defect dynamics under irradiation. This multiscale approach offers promising prospects for the predictive design of radiation-tolerant ceramic materials in nuclear, electronic and photocatalytic applications.

This research has been funded by the Latvian Council of Science grant No. LZP-2024/1-0406.

Keywords: Cubic Zirconia (ZrO_2), Radiation-Induced Defects, Density Functional Theory (DFT) and Machine Learning (ML), Raman spectra

P-22. Strain effect on CO_2 electroreduction at molecular dual-atom sites electrocatalysts

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The electrochemical reduction of CO_2 (CO2RR) into value-added chemicals is a promising strategy for carbon-neutral energy storage and utilization. Formic acid (HCOOH) is an attractive product due to its high volumetric energy density, ease of storage and transport, and wide applicability as a chemical feedstock and hydrogen carrier. However, achieving high selectivity and efficiency toward formic acid remains challenging due to competing reaction pathways and the complexity of multi-electron transfer processes. Optimizing the adsorption energies of key reaction intermediates is critical for enhancing CO_2-to-formic acid selectivity, driving efforts to tailor the electronic properties of active sites.

Here, we investigate strain-dependent electrochemical CO_2 reduction to formic acid using molecular catalysts supported on carbon materials with tunable structural properties. By systematically varying the structural characteristics of the carbon supports, we aim to elucidate how local strain and support-induced electronic effects influence catalytic performance and reaction pathways toward formic acid formation.

Key performance metrics, including Faradaic efficiency, partial current density toward formic acid, overpotential, and operational stability, will be correlated with support structure and active-site density. This experimental study clarifies whether strain enhances cooperative effects in dual-atom site systems, stabilizes key intermediates, and lowers activation barriers.

By explicitly linking strain effects to activity and reaction mechanism, this work aims to establish structural tuning of carbon supports as a versatile design strategy and to provide fundamental insights for the development of next-generation electrocatalysts capable of selective CO_2-to-formic acid conversion.

Keywords: CO_2, Density Functional Theory (DFT) and Machine Learning (ML), Electrocatalysts

Funding: This research was supported by the National Research Program BioPhoT through the project "Molecular Catalyst Design to Electrolyzer Assembly for Electrocatalytic Conversion of CO_2 to Formic Acid" (Nr. OSI_PIP_BioPhoT-2025/2-0069), carried out at the Institute of Solid State Physics, University of Latvia.

P-23. Defect-driven luminescence changes in LYSO:Ce under swift heavy ion irradiation

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Understanding the radiation response of scintillators is crucial for their application in high-radiation environments. Lutetium–yttrium oxyorthosilicate (LYSO, $Lu_{2-2x}Y_{2x}SiO_5$) doped with Ce^{3+} ions is a widely used scintillation material due to its high light yield, fast decay time, and excellent radiation hardness, making it highly suitable for medical imaging and high-energy physics applications. In this work, we investigate the effects of swift heavy ion irradiation on the luminescence properties of Kinheng LYSO:Ce single crystals using low-temperature spectroscopic techniques. The pristine crystal exhibits well-defined excitation and emission characteristics typical of Ce^{3+}-doped silicate scintillators. At 9 K, the excitation spectrum is dominated by a pronounced band near 6.7 eV, corresponding to the 4f–5d$_1$ transition of Ce^{3+} ions, indicating high crystalline quality. The emission spectrum shows two narrow bands in the blue region (396–433 nm), attributed to 5d→4f transitions to the $^2F_{5/2}$ and $^2F_{7/2}$ levels, confirming the optical purity of the material.

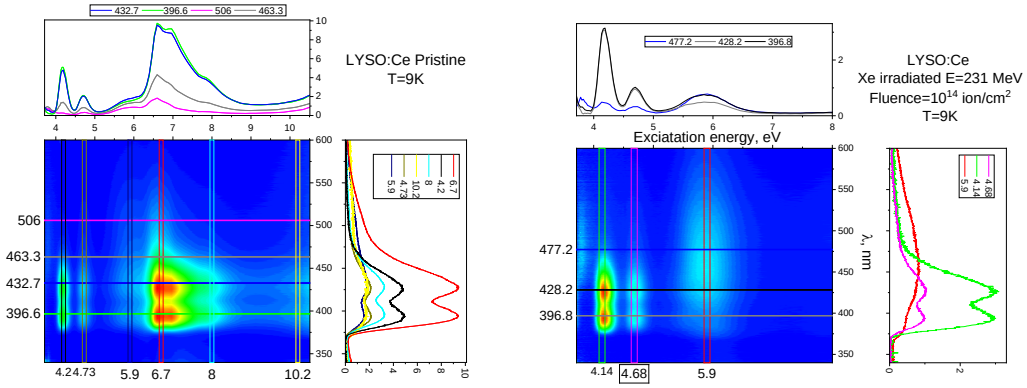

Figure 1: *3D excitation–emission maps of LYSO:Ce single crystal: pristine sample (left) and Xe-ion-irradiated sample (right, fluence F = 1 × 10¹⁴ ions/cm², energy E = 231 MeV).*

After irradiation with 231 MeV Xe ions at a fluence of 1 × 10¹⁴ ions/cm², significant spectral changes are observed. A new broad emission band centered around 450 nm appears, attributed to radiation-induced defect centers, likely oxygen vacancies or defect complexes. Concurrently, the intensity of Ce^{3+} emission decreases, indicating quenching due to irradiation-induced disorder. The excitation spectrum also shows suppression of the Ce-related band and enhanced absorption in the 4–5 eV range, suggesting the formation of defect-related excitation pathways. These results provide insight into defect formation mechanisms and their impact on scintillation performance under extreme irradiation conditions.

This research has been funded by the Latvian Council of Science grant No. lzp-2023/1-0453.

Keywords: luminescence, ion-irradiation, defects, VUV

P-24. Influence of gallium content on emission properties of $Y_3(Al_{1-x}Ga_x)_5O_{12}$:Ce scintillators

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Emerging high-energy physics applications of scintillation detectors require fast timing capabilities. The scintillation response in mature scintillator Ce-doped yttrium aluminum garnet (YAG:Ce) is limited due to charge carrier trapping at shallow defect levels. Partial substitution of aluminum with gallium in the YAG lattice mitigates these trap-related drawbacks through band-gap engineering. In this work, a detailed study was conducted to determine the limits of acceleration of scintillation decay in YAG:Ce garnets by optimizing the substitution of Al by Ga.

A set of eight $Y_3(Al_{1-x}Ga_x)_5O_{12}$:Ce (YAGG:Ce) single crystals with gallium content ranging from 0 to 1 were grown using Czochralski method in iridium crucibles on a seed with [111] orientation. Their optical properties were characterized by photoluminescence (PL), time-resolved PL (TRPL), cathodoluminescence (CL), and quantum yield (QY) measurements. A femtosecond Yb:KGW laser equipped with an optical parametric amplifier was used for resonant excitation to $5d^1$ and $5d^2$ levels of Ce^{3+} ion. PL spectra were recorded using a CCD detector, whereas the decay kinetics were measured by time-correlated single-photon counting. QY was determined using a 6-inch integrating sphere. CL measurements were performed under pulsed 10 kV electron-beam excitation using a Chronos spectrometer (Attolight) with 100 ps temporal resolution.

The temperature dependences of the PL intensity and decay time indicate that increasing gallium content in YAGG:Ce narrows the energy gap between the emitting Ce^{3+} $5d^1$ level and the bottom of the conduction band, thereby lowering the barrier for thermal depopulation and enhancing thermal quenching. Furthermore, the rise of luminescence intensity at room-temperature demonstrates that the influence of trapping centers is effectively mitigated even at a low gallium content of $x = 0.16$. At intermediate gallium contents ($x \leq 0.66$), the observed rise in quantum yield is attributed to the conversion of "dark" cerium ions into emitting Ce^{3+} centers. For higher gallium contents ($x > 0.66$), the temperature dependence of PL intensity deviates from the single-barrier Arrhenius behavior, indicating the presence of additional thermal quenching channels. Analysis of the CL measurements shows that the timing response of YAGG:Ce scintillators becomes faster with increasing gallium content up to $x \approx 0.7$. It is demonstrated that the Ga content in YAGG:Ce scintillators can be optimized based on the trade-off between emission intensity and decay time.

Keywords: scintillator, garnets, photoluminescence, cathodoluminescence, decay time

P-25. Photoelectron emission from MgO–SiO_2–Si multilayer structures at different temperatures

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MgO is a wide-bandgap dielectric with exceptional radiation hardness and thermal stability. It is used in optical windows, scintillators, and luminophores. Nanocrystalline MgO films have a high density of low-coordinated surface sites that promote the formation of surface F_s and F_s^+ color centers (oxygen vacancies). Photoelectron emission (PE) spectroscopy can be used to directly probe the energy levels of these defects relative to the vacuum level. Charge transfer (CT) between MgO defect centers and electron traps in the underlying SiO_2 layer may further influence the PE response of MgO-SiO_2-Si multilayer structures.

Nanocrystalline MgO films with a crystallite size of ~16 nm (confirmed by XRD) were deposited onto thermally oxidized Si wafers with a 1 μm SiO_2 layer via precursor pyrolysis at 550 °C. Photoelectron emission spectra (PES) of the MgO-SiO_2-Si structures were measured in a custom photothermostimulated vacuum spectrometer (10^{-3} Pa) using a 30 W deuterium lamp (4.2–6.0 eV) at room temperature (20 °C) and at 550 °C.

At room temperature, PES of MgO exhibited a low intensity, featureless spectral shape. The electron work function was 4.80 eV, consistent with direct photoemission and indicating no shallow oxygen vacancy levels near the conduction band. Heating to 550 °C increased PES intensity by over two orders of magnitude and reduced the work function to 4.19 eV. This is attributed to an Auger-assisted mechanism: (1) UV photons excite electrons from F_s and F_s^+ centers into the conduction band; (2) these electrons recombine with thermally populated V centers; (3) the energy released by this recombination is transferred non-radiatively to other electrons, which are then ejected into vacuum. Theoretical emission currents based on statistical thermodynamics agree with experimental values within an order of magnitude.

At 550 °C, distinct peaks appeared in PES, shifted ~0.2 eV to lower energies relative to the SiO_2-Si reference. We attribute this to CT from thermally populated MgO V centers to SiO_2 electron traps, followed by Auger-assisted photoemission, analogous to CT reported in Si_3N_4-SiO_2 structures [1]. The 0.2 eV shift is consistent with the dipole-induced modification of the Si–O–Si bond angle by polar groups introduced during MgO deposition.

Keywords: MgO, photoelectron emission, defect centers, Auger mechanism, SiO_2 traps

P-26. On the location of Cu^{2+} in TLD-100H

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TLD-100H, with composition LiF:Mg,Cu,P, is a well-established, highly sensitive thermoluminescence radiation detector used in personal dosimetry [1]. It has been established that all dopant elements must be present in appropriate concentrations to achieve high radiation sensitivity [2]. While this requirement is well supported by previous studies, the individual roles of each dopant and the influence of the microstructure are not yet fully clarified [3,4].

LiF:Mg,Cu,P is known to exhibit an intense Cu^{2+}-related EPR spectrum at room temperature, independent of irradiation [3–5]. Its large linewidth and lack of hyperfine structure are indicative of magnetic interactions between Cu^{2+} ions. However, a detailed understanding of the location of Cu^{2+} in the dosimeter and its role in the dosimetric response is still missing. In this work, we combine X- and Q-band Electron Paramagnetic Resonance (EPR) with X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM) coupled to cathodoluminescence to address this knowledge gap. XRD and SEM show that P- and O-rich phases are present in the dosimeter material, separated from the main LiF phase. In this presentation, we explore different synthesis routes and compare their spectroscopic characteristics with those of the TLD-100H dosimeter.

Keywords: Electron Paramagnetic Resonance, Radiation Dosimetry, Dopant Microstructure.

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P-27. Sustainable synthesis of carbon-based luminescent materials from biomass waste via thermal plasma processing

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Thermal plasma treatment represents a versatile approach for tailoring structural, morphological and defect-related properties of materials under extreme thermochemical conditions. Beyond conventional inorganic systems, this work emphasizes the transformation of biomass-derived feedstocks into functional carbon-based nanomaterials. In particular, organic waste materials, such as tomato residues and other biomass/polymer-type wastes, are processed via thermal plasma to produce carbon-rich nanoparticles with tunable structural and surface properties. The plasma environment enables rapid decomposition, carbonization and restructuring of the organic precursors, leading to the formation of nanostructured carbon materials. These carbon nanoparticles can subsequently serve as precursors for the synthesis of carbon quantum dots (CQDs), whose optical properties can be precisely tuned through control of processing conditions and post-treatment steps. The resulting CQDs exhibit promising photoluminescent behavior and can be further engineered for advanced optical applications. A key focus of this study is the development of luminescent materials based on CQDs, including their potential use in upconversion processes. Such materials are of particular interest for applications in photonics, sensing and energy-related technologies. The influence of plasma treatment on the structure, defect states and optical response of the synthesized materials is investigated using complementary structural and spectroscopic techniques. The results highlight the potential of thermal plasma processing as a sustainable and flexible tool for converting low-value biomass waste into high-value functional nanomaterials, enabling new pathways for the design of carbon-based luminescent systems with advanced optical functionalities.

Keywords
thermal plasma, biomass upcycling, tomato waste, carbon nanoparticles, carbon quantum dots, upconversion luminescence, defect engineering, circular economy

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P-28. Host-dependent structure–properties correlations in rare earth-doped CaF_2 and BaF_2 crystals

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Fluoride hosts doped with Rare-Earth (RE) ions offer opportunities for many domains as they are potential candidates in luminescent, dosimetric, and photochromic applications, owing to their low phonon energies, wide optical transparency in UV-VIS-NIR range, and relatively inert chemical environment [1-4]. The MF_2 fluoride materials crystallize into a cubic structure (Fm-3m space group) characterized by M^{2+} cations surrounded by eight F^- ions, F^- atoms enclosed by four M^{2+} ions and can accept a wide variety of ions, both bivalent and trivalent, due to the same number of octahedral interstitial sites (positions) as the number of M^{2+} ions. The RE^{3+} doping into the host lattice is made without change in the symmetry and the excess of charge is compensated by interstitial F^- ions leading to different isolated site symmetry centers depending on the RE^{3+} concentrations i.e. at low RE^{3+}: tetragonal (C_{4v}), trigonal (C_{3v}) or cubic (O_h) or complex clusters for higher RE^{3+} doping. CaF_2 and BaF_2 materials tolerate RE substitution while preserving good crystal quality and enhanced properties. In order to analyse the influence of RE (RE=Er, Tm or Tb) doping upon structural, morphological and optical properties of MF_2 (M=Ca or Ba) matrix, single crystals were grown by using the vertical Bridgman-Stockbarger method [5] and characterised by X-Ray and neutron diffraction on single crystal or crushed single crystals. The interplay between the local lattice distortions correlated with charge compensation mechanism induced by doping and the observed properties (morphology: defects evolution, absorption bands associated with divalent and trivalent doping RE ions [6]) are discussed in the work.

Keywords: fluoride, crystal structure, doping.

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P-29. Radiation-induced Tm^{2+} ions and thermal oxidation in Tm-doped alkaline-earth fluoride crystals

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Fluoride hosts doped with Rare-Earth (RE) ions offer compelling advantages for luminescent, dosimetric, and photochromic applications, owing to their low phonon energies, wide optical transparency in UV-VIS-NIR range, and relatively inert chemical environment [1-2].Various concentration of TmF_3-doped calcium and barium fluoride crystals were grown using the vertical Bridgman-Stockbarger method [3]. Cleaved disks of 10mm diameter and 1 mm thickness from the as-grown single crystals were irradiated at Room Temperature (RT) under continuous X-Ray at different intervals of 1h, 2h, 3h and 4 h. Optical absorption spectra at room temperature of non-irradiated CaF_2 single crystals present distinct features associated with Tm^{3+} and Tm^{2+} ions, whereas for BaF_2 samples only bands associated with Tm^{3+} ions were observed. The intensity absorption bands present a dependence on the TmF_3 concentration and on the matrix type (CaF_2 or BaF_2). Following the X-Ray irradiation, a change of the absorption spectra was observed in the UV-VIS region. The X-Ray irradiation induces the enhancement of Tm^{2+} absorption bands, indicating an efficient $Tm^{3+} \rightarrow Tm^{2+}$ charge conversion process in both hosts (CaF_2 and BaF_2). Thermal annealing up to temperatures of 600°C was further performed in order to investigate the mechanisms involved in Tm^{2+} to Tm^{3+} oxidation and their impact on the spectral properties. Luminescence measurements were carried out to assess the influence of X-Ray irradiation and thermal annealing on the emission properties of these Tm-doped fluorides. This study shed light on how X-Ray ionizing radiation influences the optical behavior of Tm-doped alkaline-earth fluoride crystals, emphasizing their promise for use in radiation detection and similar technological applications.

Keywords: fluoride, X-Ray irradiation, Optical absorption, charge conversion.

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P-30. Symmetry environment of europium in $NaMgF_3$ fluoroperovskite: A combined XANES, EXAFS and atomistic modeling study

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Europium-doped fluoroperovskite $NaMgF_3$ was investigated concerning the site occupancy of the dopant, its valence state, and the resulting influence of these features on the luminescent emission of the doped material. While previous studies have focused primarily on optical spectroscopy to infer dopant environment, the present work provides a direct investigation about local order using X-ray Absorption Fine-Structure (XAFS) combined with atomistic computational modelling. Eu-doped $NaMgF_3$ samples were synthesized via the microwave-assisted hydrothermal method (MAHM). XANES analysis demonstrated that Eu ions coexist in both 2+ and 3+ oxidation states. These results were considered in atomistic computational modelling of defects which predicts 2+ and 3+ species substituting Na^+ site with $Na^{'}_{Mg}$ anti-site defects to compensate charge disbalance. This structural model corroborates with EXAFS fitting which successfully described the coordination environment of the dopant. These results
contribute to elucidate some ambiguities in literature about lanthanide doping for this material.

Keywords: Fluoroperovskites, XAFS, Classical atomistic modelling, defects

P-31. Crystal growth and characterization of KTb_3F_{10} single crystal

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Magneto-optical materials are essential components in optical isolators based on the Faraday effect, and they play a critical role in high-power solid-state laser systems. In particular, terbium-based single crystals offer several advantages, including a wide optical transparency range, low absorption, and high thermal stability. They also operate effectively across the ultraviolet (UV), visible (VIS), and near-infrared (NIR) spectral regions.

Among these materials, KTF (KTb_3F_{10}) crystals are especially attractive because they exhibit low nonlinear refractive indices and small thermo-optic coefficients, while still providing Verdet constants comparable to those of TGG - the most widely used magneto-optic crystal in industry. However, unlike TGG, KTF melts incongruently, making its crystal growth significantly more challenging.

This poster presents the growth of KTb_3F_{10} single crystals, along with their structural characterization (XRD and Laue), spectroscopic properties, and measured Verdet constants.

Keywords: KTF, magneto-optic, single crystal

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P-32. DFT modeling of elastic properties of m-ZrO_2

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This study presents the results of an investigation of the elastic, mechanical, and electronic properties of the monoclinic phase of zirconium dioxide, m-ZrO_2, under hydrostatic pressure in the range of 0–20 GPa. The elastic characteristics were calculated based on 13 independent elastic constants using the Voigt–Reuss–Hill approximation, which is commonly applied for evaluating the elastic properties of monoclinic ZrO_2 [1,2]. It is shown that with increasing pressure, most elastic constants increase, indicating enhanced rigidity of the crystal lattice and greater resistance to deformation. The bulk modulus increases from 162.20 to 209.50 GPa, Young's modulus from 221.69 to 273.66 GPa, and the shear modulus from 87.13 to 106.71 GPa. The results indicate that m-ZrO2 remains mechanically stable throughout the pressure range investigated.

The analysis of Cauchy constants and the universal anisotropy index shows that the elastic response of the monoclinic structure is strongly anisotropic. The anisotropy index changes non-monotonically: it first decreases from 2.52 at 0 GPa to a minimum value of about 1.06 at 10 GPa and then increases again to 1.40 at 20 GPa. The B/G ratio lies in the range of 1.76–2.09, suggesting a transitional behavior between brittle and more ductile characteristics. The Poisson's ratio varies within 0.262–0.294, indicating the preservation of moderate ductility. In addition, the band gap increases from 5.4942 to 6.1828 eV, which indicates an enhancement of the dielectric properties of m-ZrO_2 under pressure and agrees with the importance of electronic-structure analysis for zirconia-based materials [3].

The results obtained demonstrate that hydrostatic pressure promotes an increase in stiffness, strength characteristics, and dielectric properties of monoclinic ZrO_2. At the same time, the material maintains mechanical stability and retains the anisotropic nature of its elastic properties.

Keywords: DFT, zirconium dioxide, pressure, monoclinic phase, mechanical properties

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P-33. Effect of pressure and temperature on the luminescent properties of Cu- and Mn-activated hydroxyapatite

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Hydroxyapatite is a promising biomaterial due to its chemical similarity to the mineral component of bone tissue and tooth enamel, while its doping with transition metal ions makes it possible to modify its structural, physicochemical, and optical properties. Recent studies show that the introduction of Cu ions into the hydroxyapatite structure affects the crystal lattice parameters and crystallinity of the material and can also improve its functional and biomedical characteristics [1]. For Mn-doped hydroxyapatite, the influence of manganese on the crystal structure and biocompatibility of the material has also been demonstrated [2]. In addition, studies of Cu-containing hydroxyapatites confirm the importance of investigating luminescence processes, since Cu^{2+} ions can significantly affect emission intensity and luminescence quenching mechanisms [3].

In this work, the effect of pressure and temperature on the luminescent properties of pure, copper- and manganese-activated hydroxyapatite was studied. The objects of the study were pure hydroxyapatite, Cu-HAp, and Mn-HAp; the aim of the work was to investigate changes in luminescence intensity depending on pressing and heating conditions. Experimental studies were carried out using scanning electron microscopy, X-ray diffractometry, and spectrofluorimetry; excitation and emission spectra were obtained at different pressures and temperatures.

It was established that Cu-HAp and Mn-HAp show a similar pressure-dependent behavior of luminescence intensity at 300 K and 423 K. When recording excitation spectra, the intensity increased at pressures of 2.5 and 7 MPa, while a decrease was observed at 5 MPa. When recording emission spectra, on the contrary, an increase in intensity was observed at 5 MPa, whereas at 2.5 and 7 MPa the intensity decreased. Temperature studies showed that heating the samples leads to a sharp decrease in luminescence intensity; it was also noted that samples pressed at high pressure exhibit weaker luminescence, therefore lower pressing pressures are preferable for maintaining emission intensity.

The obtained results show that pressing pressure and temperature are important factors determining the luminescent response of Cu- and Mn-activated hydroxyapatite. This can be used in the development of functional biomaterials and optically active systems based on modified hydroxyapatite.

Keywords: hydroxyapatite, Cu-HAp, Mn-HAp, luminescence, pressure, temperature, spectrofluorimetry, biomaterials.

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P-34. Optical and magnetic spectroscopy investigations of sol-gel derived Cr^{3+}-doped Ga_2O_3 nanoparticles

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Recently, chromium (III) doped β-Ga_2O_3 has been proposed as a promising material for high-efficiency broadband near-infrared (NIR) light sources and imaging applications [1].

We used the sol-gel citrate method to prepare Cr^{3+}(1 mol%)-doped β-Ga_2O_3 nanocrystals and performed a correlative study of their structural, magnetic, and photoluminescence properties. Thermal analysis showed complex decomposition of the intermediate crystalline phases up to 800 °C, at which the nanocrystals form. The X-ray diffraction pattern analysis and scanning electron microscopy investigations revealed the formation of nanocrystals with sizes on the order of tens of nm. According to electron magnetic resonance (EPR) investigations, the Cr^{3+} ions substitute for Ga^{3+} ions, likely at an octahedral Ga^{3+} site, with a trigonal distortion [2]. The XPS spectroscopy indicated the occurrence of Cr^{6+} ion species caused by partial oxidation of Cr^{3+} to Cr^{6+} ion species during the air calcination. Under Cr^{3+} ion blue-light excitation at 445 nm ($^4A_2 \rightarrow {}^4T_1$), the photoluminescence spectrum shows two sharp R-lines at 688 and 696 nm ($^2E \rightarrow {}^4A_2$), accompanied by a broad band peaking at about 705 nm ($^4T_2 \rightarrow {}^4A_2$) [3]. Thermoluminescence measurements revealed the presence of low-energy trap levels associated with Cr^{3+} doping and responsible for the room-temperature afterglow luminescence. A polymeric dispersion of the nanocrystalline powder was tested to observe and photograph infrared-luminescent writing with a commercial smartphone, demonstrating promising properties for security printing applications and luminescent QR code labelling.

Keywords: nanocrystals, infrared phosphor, thermoluminescence

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P-35. Morphological modification of TiO_2/Ag nanostructure-coated macroporous silicon under high-energy heavy-ion irradiation

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Macroporous silicon coated with photocatalytic and plasmonic nanostructures is a promising platform for self-cleaning filters and highly sensitive surface-enhanced Raman scattering (SERS) sensors. Structural modification using swift heavy-ion irradiation provides an effective route for tailoring pore morphology and defect density, thereby improving functional performance.

In this work, the morphology of macroporous silicon (macroPSi) coated with a TiO_2 thin film (100 nm) and Ag nanoparticles (AgNPs) was investigated after irradiation with high-energy Ar^{8+} and Xe^{22+} ions. Ion bombardment resulted in significant restructuring of the near-surface region due to ion-track formation. Xe^{22+} irradiation produced stronger morphological changes compared to Ar^{8+} irradiation, leading to pronounced pore widening and deepening. The average equivalent pore diameter increased by 14% and 40% after Ar^{8+} and Xe^{22+} irradiation, respectively.

Elemental analysis revealed a decrease in Si and Ti content after Xe^{22+} irradiation accompanied by an approximately 15% increase in oxygen concentration, indicating oxidation of the silicon matrix and partial damage to the TiO_2 layer near pore edges. In samples containing AgNPs, irradiation resulted predominantly in surface smoothing rather than pore deepening. This effect is attributed to enhanced energy dissipation caused by interaction of heavy ions with Ag nanoparticles characterized by a high density of dangling bonds. Nevertheless, significant widening of pore necks was observed, with diameter increases of 15% and 28% after Ar^{8+} and Xe^{22+} irradiation, respectively.

Xe^{22+} ions additionally modified the silicon skeleton density through ion-track formation, while both ion species reduced the Ti/Ag atomic content. Overall, high-energy heavy-ion irradiation introduces structural defects and compositional changes that can enhance photocatalytic efficiency and SERS sensitivity, opening prospects for antibacterial applications and ultrasensitive molecular detection.

Keywords: Swift heavy-ion irradiation, Macroporous silicon, Photocatalytic and plasmonic nanostructures.

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P-36. Optical and structural modifications of $MgAl_2O_4$ single crystals under swift heavy-ion irradiation

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Magnesium aluminate spinel ($MgAl_2O_4$) is one of the most radiation-resistant dielectric oxides, making it a promising material for nuclear energy applications and radiation-tolerant optical components. Understanding the formation of irradiation-induced defects and their influence on optical properties is essential for predicting the performance of spinel-based materials in extreme environments.

In this work, the effect of 220 MeV Xe swift heavy ions on the structural and optical properties of $MgAl_2O_4$ (111) single crystals was investigated. Irradiation experiments were performed using the DC-60 cyclotron (Astana, Kazakhstan) in order to simulate the impact of energetic fission fragments on the crystal lattice. Optical absorption, photoluminescence (PL), photoluminescence excitation (PLE), and depth-resolved confocal Raman spectroscopy were employed to characterize defect formation and structural modification along the ion trajectory.

The irradiated crystals exhibit a broad absorption band centered at approximately 5.3 eV attributed to F^+ and F-type color centers, while hole-related defects contribute to absorption in the 3–4 eV spectral range. The material remains transparent in the near-infrared region, indicating preservation of its dielectric properties despite irradiation-induced damage.

Raman spectroscopy revealed the presence of additional vibrational modes A1g* (720 cm^{-1}) and Eg* (385 cm^{-1}), appearing as asymmetric features near the main Eg mode. The intensity of the Eg Raman mode increases with probing depth and reaches a maximum at approximately 13 μm, remaining nearly constant up to the projected ion range (~14 μm). Progressive broadening of the Raman band near 408 cm^{-1} indicates increasing structural disorder and partial amorphization along the ion track. The obtained results suggest that irradiation with high-energy Xe ions induces cation disorder and defect-related optical centers while preserving overall transparency of the material.

These findings confirm the high radiation tolerance of $MgAl_2O_4$ spinel and demonstrate its potential for applications in radiation-resistant optical materials and nuclear technologies.

Keywords: Swift heavy-ion irradiation; $MgAl_2O_4$ spinel; Radiation-induced defects

P-37. Radiation-induced defect formation and optical property modification in $Y_3Al_5O_{12}$ single crystals irradiated with Xe and N ions

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Yttrium aluminum garnet ($Y_3Al_5O_{12}$, YAG) is an important wide band-gap material widely used as a host matrix for rare-earth dopants in solid-state lasers, scintillators, phosphors, and radiation detectors. Its high radiation stability and ability to accommodate intrinsic defects make YAG promising for applications operating in harsh radiation environments. However, irradiation induces structural and electronic defects that significantly influence optical and mechanical properties. Understanding the mechanisms of radiation-induced defect formation is therefore essential for improving radiation resistance and tailoring functional properties of YAG-based materials.

In this work, structural and optical properties of YAG single crystals irradiated with 230 MeV Xe ions and 24.5 MeV N ions were comparatively investigated using optical absorption spectroscopy, photoluminescence spectroscopy under synchrotron radiation excitation, Raman spectroscopy, nanoindentation measurements, and high-resolution transmission electron microscopy (HRTEM). The study focuses on the role of electronic stopping power in defect formation and modification of luminescent properties. Irradiation with high-energy Xe ions is characterized by high electronic energy loss (Se = 25.2 keV/nm), exceeding the threshold for track formation in YAG. HRTEM analysis revealed formation of latent ion tracks with an amorphous core of approximately 5 nm in diameter surrounded by a damaged region of about 10 nm. Increasing fluence leads to track overlap, partial amorphization of the near-surface layer, and significant softening of the material, with hardness reduction up to 60% at fluence 10^{13} ions/cm^2. Optical absorption spectra demonstrate formation of radiation-induced color centers associated with oxygen vacancies (F and F^+ centers) and antisite defects. Photoluminescence measurements show increased emission intensity of F-type centers in the spectral region around 400–460 nm, indicating increased concentration of oxygen vacancies.

In contrast, irradiation with 24.5 MeV N ions (Se ≈ 1.94 keV/nm) does not reach the threshold for track formation and mainly produces point defects and defect complexes without significant amorphization. Raman spectroscopy confirms progressive lattice disorder for Xe irradiation, while only minor structural modifications are observed for N irradiation.

The results demonstrate that radiation damage mechanisms in YAG strongly depend on electronic stopping power. Ion irradiation can be used as a controlled method for modification of defect structure and optical properties of YAG crystals for advanced photonic and radiation detection applications.

Keywords: $Y_3Al_5O_{12}$ (YAG); ion irradiation; radiation defect

P-38. A peculiar photoluminescence behavior of F_3^+ color centers in lithium fluoride crystals irradiated with gamma rays at low doses

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Lithium fluoride (LiF) crystals were irradiated at three clinical doses of 5, 10 and 20 Gy with gamma rays of the ^{60}Co primary beam at the Italian National Institute of Ionizing Radiation Metrology. The irradiations created optically-active point defects in the LiF lattice, among which the aggregate $F3^+$ color centers (CCs). A recent accurate analysis of the green photoluminescence (PL) band at increasing excitation power of a 445 nm laser, in stationary conditions [1], had not only suggested the presence of an emission band overlapped with the $F3^+$ one, that might be ascribed to F3 (R2) defects, but had also allowed estimating a parameter of the $F3^+$ energy triplet state, whose value well agreed with the literature [2].

The presence of the triplet state in the optical cycle of the $F3^+$ CCs causes its PL quenching, taking place as soon as the pump laser is switched on, reaching a stationary intensity after several seconds, depending on the laser power. The time dependence of the $F3^+$ CCs PL intensity has been studied in the first seconds of laser pumping, until the stationary condition is reached. It has shown a time evolution that can be described by the superposition of two contributions with different exponential decay times. In this presentation, the analysis of the PL spectra will be shown with a tentative explanation of this observed peculiar unexpected behavior.

Keywords: lithium fluoride, $F3^+$ color center, triplet state.

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P-39. Radiophotoluminescence of F_2 color centers in lithium fluoride crystals for dosimetric evaluations in proton irradiation of Antarctic cryptoendolithic communities for the CRYPTOMARS project

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The CRYTPOMARS project [1], funded by the Italian Space Agency (ASI contract n. 2023- 12-U.0), is a multidisciplinary research project aimed at investigating, with a multi-omic approach, the mechanisms of resistance developed by Antarctic cryptoendolithic communities, microbial assemblages living in the airspaces of porous sandstones, including those from the McMurdo Dry Valleys (ice-free areas of Continental Antarctica). These communities, exploiting the refuge provided by the rock, survive in an environment referred to as "Martian analogue on Earth". Investigation of their metabolic properties has been conducted after exposing colonized samples of Antarctic rocks, separately, to different stress factors representative of the Martian environment, such as thermal and hydration/dehydration cycles, UV and ionizing radiation.

In this presentation, we report the experimental set-up design, the dosimetric characterization and beam monitoring result of the irradiation campaign with the 71 MeV proton beam, provided by the TOP-IMPLART linear accelerator at ENEA Frascati Research Centre [2], that was performed by exploiting the red radiophotoluminescence of radiation-induced F_2 color centers in lithium fluoride crystals, allowing to evaluate also the radiation shielding effect of the microbial communities.

Keywords: lithium fluoride, dosimetry, Antarctica.

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P-40. Self-trapped exciton emission in natural quartz: effects of structural disorder and temperature on radioluminescence

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In this study, radioluminescence (RL) spectra of natural quartz grains were measured over a temperature range of 8-300 K using samples derived from diverse geological settings with crystallisation ages spanning from Ma to Ga. The investigated quartz grains include two granites, one metamorphosed granite, and two sedimentary samples. The RL spectra exhibit a dominant blue emission band at ~2.6 eV below 200 K, attributed to self-trapped exciton (STE) emission, which disappears at higher temperatures.

Analysis of RL intensity as a function of temperature (50-150 K) using an Arrhenius model yields activation (quenching) energies in the range of 24-53 meV. The variation of full width at half maximum (FWHM) with temperature was modelled using Toyozawa electron-phonon coupling model and the Bose-Einstein phonon coupling model to estimate phonon energies. Compared to synthetic quartz reported in the literature, natural quartz samples show broader FWHM and earlier quenching, reflecting a higher degree of structural defects and disorder. Significant variations in emission characteristics, including relative intensity, peak position, FWHM, quenching behaviour, and phonon energies, are observed among samples from different geological environments. Deformed samples exhibit broader emission bands, lower quenching energies, and lower phonon energies, indicating reduced exciton stability.

These results confirm the presence of exciton-related recombination processes in natural quartz and demonstrate that STE emission is highly sensitive to structural disorder, impurity content, and the geological history of the samples.

Keywords: Radioluminescence, natural quartz, self-trapped exciton (STE), phonon energy, quenching energy, structural disorder.

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P-41. **Integrating Experimental Spectroscopy and Machine Learning for Predicting Pr^{3+} 5d Levels in UV-C and UV-B Oxide Upconversion Phosphors**

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The development of efficient ultraviolet (UV) phosphors is essential for environmentally friendly UV light sources, particularly as conventional mercury-based lamps are being phased out and semiconductor UV emitters remain limited by low conversion efficiencies. Pr^{3+}- activated oxide hosts are promising candidates for UV-C and UV-B emission owing to the parity-allowed $4f^2 \rightarrow 4f^1 5d^1$ transitions.

In this work, the lowest Pr^{3+} 5d absorption and emission levels were experimentally investigated in Lu_2SiO_5, YBO_3, $YAlO_3$, $La(PO_3)_3$, and Y_2O_3 and compared with machinelearning (ML) predictions. The lowest 5d absorption and emission bands were found between 215−350 nm and 240−350 nm, respectively. Visible-to-ultraviolet upconversion was observed only in YBO_3^{3+} and $Lu_2SiO_5^{3+}$, with YBO_3^{3+} exhibiting the strongest UV-C emission and $Lu_2SiO_5^{3+}$ predominantly emitting in the UV-B region.

A Random Forest model trained using crystallographic descriptors from the Materials Project database was applied to approximately 20000 inorganic compounds, as shown in [1] . Band gap, coordination number, cation−anion distance, and local bond-angle geometry were identified as the most influential descriptors. The optimized models achieved mean absolute errors of 7.12 nm for absorption and 5.79 nm for emission, showing excellent agreement between predicted and experimental Pr^{3+} 5d levels. The combined experimental−ML approach provides an efficient strategy for accelerating the discovery of Pr^{3+}-activated oxide phosphors for potential ultraviolet applications.

Keywords: VIS to UV-C upconversion, optical materials, integration PL - ML.

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