RÅC INTERNATIONAL SUMMER SCHOOL 2025

Advanced Materials Design at X-ray and Neutron Facilities

RÅC International
Summer School

Secretariat, *c/o DESY*
Notkestraβe 85
22607 Hamburg

E-mail: rac-school@desy.de
Tel: +49 40 8998 4172

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Advanced Materials Design at X-ray and Neutron Facilities

Diffraction and Spectroscopy in Materials Science

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a.kuzmin@cfi.lu.lv

Tuesday, 26.08.2025, 14:00-15:00

Alexei Kuzmin

Head of the Laboratory

Institute of Solid State Physics, University of Latvia

Kengaraga street 8, LV-1063 Riga, Latvia

Fields of interest:

X-ray absorption spectroscopy, Computer simulations, Functional materials

AI in Spectroscopy

The evolution of X-ray absorption spectroscopy has been shaped by advancements in experimental capabilities, computational methodologies, data analysis techniques, and interdisciplinary applications. Although the theoretical foundations of X-ray absorption spectra are well-established, their interpretation remains complex due to the ill-posed nature of the problem [1]. Processing large datasets from high-throughput or time-resolved experiments is also particularly demanding, especially in real-time applications. Emerging machine learning methods are expected to help address these challenges and will be the focus of this lecture. The state of the art and the role of AI-based approaches among existing methods will be presented. In particular, the use of machine learning potentials and artificial neural networks for predicting X-ray absorption spectra from atomic structures (the forward problem) [2], as well as reconstructing atomic structures from spectra (the inverse problem) [3], will be discussed.

[1] A. Kuzmin, in High-Entropy Alloys: Design, Manufacturing, and Emerging Applications, G. Yasin, M. Abubaker Khan, M. Afifi, T. Anh Nguyen, Y. Zhang (Eds.), pp. 121-155 (Elsevier, 2024).
[2] P. Žguns, I. Pudza, A. Kuzmin, J. Chem. Theory Comput., 2025, doi: 10.1021/acs.jctc.5c00955.
[3] J. Timoshenko, A. Anspoks, A. Cintins, A. Kuzmin, J. Purans, A.I. Frenkel, Phys. Rev. Lett., 2018, 120, 225502.

Short Biography

Dr. A. Kuzmin is the Head of the EXAFS Spectroscopy Laboratory at the Institute of Solid State Physics, University of Latvia. He received his Doctorate in Physics from the University of Latvia, Riga, in 1992. He specializes in X-ray absorption spectroscopy using synchrotron radiation, with a particular focus on developing advanced data analysis methods such as reverse Monte Carlo simulations, Molecular Dynamics, and Machine Learning. He has published over 300 research papers and contributed to two books. His current research interests involve studying the structure-property relationships in smart (photochromic, electrochromic, thermochromic) and multicomponent (high-entropy) materials.