Krakow School of Interdisciplinary PhD Studies <KISD>
invites PhD students and members of the research staff
to attend the series of guest lectures given by:

Prof. Pavel Korzhavyi

KTH Royal Institute of Technology, Stockholm, Sweden

Modern materials challenges: from atomistic simulations to transforming global economy

A. Thermodynamic properties from ab initio calculations as input to Calphad modeling

Models that are used for linking together the different length- and time-scales relevant to materials' properties and performance are considered. The consideration is focused on discrete models at the electronic/atomistic and mesoscopic levels, as well as on their interface with the continuum level (Calphad). Some recent achievements and existing challenges will be discussed in the context of the development of universal and rigorous models for atomically-informed modelling of thermodynamic properties of materials.

B. Challenges and Opportunities for the Rare Earth Element (REE) Industry in the EU

The history of the discovery of Rare Earth elements (REE) will be briefly recalled. The focus will then be shifted to the applications of REE-based permanent magnets in our modern electrified society. The technological, economic, and societal challenges associated with the REE life cycle will be discussed.

C. Further studies of vacancies in transition metal carbides

Transition-metal carbides combine properties typical of ceramics (high hardness, melting point, chemical stability) and metals (good thermal and electrical conductivity). This combination makes them suitable for numerous applications in extreme environments (high temperatures and radiation fields) where the material's behavior is controlled by the properties of atomic defects. Ab initio calculations give us the defect formation and interaction energies, as well as the barriers for defect migration through the crystal lattice. The results of systematic ab initio studies of point defects in the group 4 and 5 transition metal carbides will be reviewed

Schedule:
A. Monday, **24.03.2025, 12:00 pm.**
IMIM PAN, ul. Reymonta 25, 30-059 Kraków
Conference room, 2nd floor

B. Wednesday, **26.03.2025, 11:00 am.**
IMIM PAN, ul. Reymonta 25, 30-059 Kraków
Conference room, 2nd floor

C. Thursday, **27.03.2025, 11:00 am.**
IMIM PAN, ul. Reymonta 25, 30-059 Kraków
Conference room, 2nd floor

Prof. Pavel Korzhavyi *is a professor at the Department of Materials Science and Engineering at the Royal Institute of Technology (KTH) in Stockholm. His expertise is in modeling disordered crystals and their thermodynamic and kinetic properties, starting from first principles of quantum mechanics. This theoretical modeling is applied to materials of industrial relevance, e.g. metals and ceramics at elevated temperatures.*
Pavel Korzhavyi is KTH's official representative in the Knowledge and Innovation Community RawMaterials at the European Institute of Innovation and Technology (EIT RawMaterials). He is the leader of ExpSkills-REM project on Expanding Knowledge and Skills in Rare Earth Permanent Magnets Value Chain, financed by the EIT RawMaterials co-funded by the European Union.

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