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

Prof. Pavel Korzhavy

Royal Institute of Technology, Stockholm, Sweden

A. Atomistic modeling of thermodynamic properties

Bonding in molecules and solids; Ground state structure and energy; Electron density and total energy; Cohesive properties; Lattice vibrations; (Quasi)harmonic: Zero-point energy; Strongly anharmonic vibrations: Ab initio molecular dynamics; Vibronic effects; Bridging ab initio and classical molecular dynamics; Pair potentials; Many-body potentials for metals and semiconductors; Reactive many-body potentials; Machine-learning potentials.

B. Atomistic modeling of defects and disorder in metals

Classification of defects and disorder in solids; Supercell approach vs. perturbation theory; Defect interactions and clustering; Selected results on point defects; Concentrated alloys; Quasi-random structures; Coherent potential approximation (CPA); Interpolation: Selected results; Paramagnetic disorder; Disordered local moment (DLM) approaches; Alloy analogy (mean field); Spin spirals and "ideal paramagnet"; Vibrational disorder; Quasi-harmonic Debye model; Alloy analogy (Einstein model).

C. Atomic and electronic structure of vacancies in transition metal carbides

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

Pavel Korzhavy *is a professor in Materials Technology at KTH Royal Institute of Technology, Stockholm, Sweden. His research is focused on modeling disordered crystals to compute their thermodynamic and kinetic properties starting from first principles (ab initio). This modeling is applied to industrially relevant materials such as metallic alloys and ceramic compounds.*

Pavel Korzhavyi is KTH's official representative in the Knowledge and Innovation Community EIT RawMaterials at the European Institute of Innovation and Technology and in the European Raw Materials Alliance. 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. Korzhavyi is a member of the advisory editorial board of the Journal of Nuclear Materials.

Schedule:

A. Monday, **20.11.2023, 1:00 - 2.30 pm.**
IFJ PAN, ul. Radzikowskiego 152, 31-342 Kraków
MSD room, 1st floor

B. Wednesday, **22.11.2023**, **9:30 - 11.00 am.**
IFJ PAN, ul. Radzikowskiego 152, 31-342 Kraków
MSD room, 1st floor

C. Friday, **24.11.2023**, **11:00 am.– 12.30 pm.**
IMIM PAN, ul. Reymonta 25, 30-059 Kraków
Conference room, 2nd floor

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