

# 6<sup>th</sup> Users' Conference of IT4Innovations

November 3 and 4, 2022 / IT4Innovations

[Paolo Nicolini](#) (Institute of Physics of the CAS): *Ultra-low friction and edge-pinning effect in large-lattice-mismatch van der Waals heterostructures*

[Prokop Hapala](#) (Institute of Physics of the CAS): *Integrated simulation package for on-surface chemistry and SPM*

[Michal Svatos](#) (Institute of Physics of the CAS): *ARC-CE+HyperQueue based submission system of ATLAS jobs for the Karolina HPC*

[Zdenek Futera](#) (University of South Bohemia): *Tunneling Conductivity of Protein/Metal Junctions Investigated by Large-Scale DFT Simulations*

[Petra Cechova](#) (Palacky University Olomouc): *Interactions of Ionizable and Membrane Lipids*

[Hugo McGrath](#) (University of Chemistry and Technology): *Binding of Peptide Deformylase to the Ribosome Surface Modulates Exit Tunnel Interior*

[Petr Rehak](#) (Brno University of Technology): *Role of entropy term on the grain boundary segregation in bcc Fe*

[Jan Ludik](#) (University of Chemistry and Technology): *Efficient pathways of quantum-chemical modelling of cohesion for crystalline pharmaceutically active ingredients*

[Ondrej Olsak](#) (Brno University of Technology): *Evaluation of libraries for the one-dimensional sparse Fourier transform*

[Damien Gagnier](#) (Charles University): *Binary evolution and angular momentum transport during common-envelope post-dynamical spiral-in phase*

[Gabriela Necasova](#) (Brno University of Technology): *Parallel solution of partial differential equations using Taylor series method*

[Matus Kaintz](#) (Czech Technical University in Prague): *Engineering Width and Directness of the Band Gap in Diamond-based Materials*

[Martin Heczko](#) (Brno University of Technology): *Mn-excess Ni-Mn-Ga alloys – First-Principles study*

[Pavel Ondracka](#) (Masaryk University): *Hard and moderately ductile orthorhombic (Mo,X)<sub>2</sub>BC alloys*

[Jan Heyda](#) (University of Chemistry and Technology): *Kirkwood-Buff theory approach towards cosolvent effects on single polymer chain collapse transition*

[Petra Kuhrova](#) (Palacky University Olomouc): *Computer folding of parallel DNA G-quadruplex*

[Petr Tous](#) (University of Chemistry and Technology): *First-principles modeling of local disorder in crystalline caged hydrocarbons and its implications to their thermodynamic properties*

[Jana Pavlu](#) (Masaryk University): *Properties of MoSi<sub>2</sub>/XSi<sub>2</sub> (X = Nb, Ta, Ti) nanocomposites from quantum-mechanical perspective*

[Miroslav Rubes](#) (IOCB of the CAS): *Modeling of zeolite properties on HPC*

[Andrzej Piotr Kądziaława](#) (IT4Innovations): *Materials for application in Fusion Reactors: Determining the elastic properties of single grains in the ultrafine-grained W-Cr composite*

[Amrit Sarmah](#) (IOCB of the CAS): *Rational Design of Photo-active Nanomaterials for Energy, Environmental, and Electronic Applications*

[Prashant Dwivedi](#) (Czech Technical University in Prague): *Molecular dynamics simulations of hypervelocity dust impacts on plasma facing materials*

[Felipe Castro Nepomuceno](#) (University of Chemistry and Technology): *Peptide Translocation in Carbon Nanotube: Pulling vs Pushing*

[Monika Všíanská](#) (Masaryk University): *A Quantum Mechanical Study of Tin Segregation at Tilt Grain Boundaries in Iron*

[Kristián Kadlubiak](#) (Brno University of Technology): *Comparison of Interpolation Methods in Non-uniform LFB Scheme*

[Marta Jaros](#) (Brno University of Technology): *k-Plan: from the Hospital to the Cluster and back*

[Petr Linhart](#) (University of Chemistry and Technology): *Conformational behaviour of the uL22 protein*