

8th Users' Conference of IT4Innovations

4 – 5 November 2024

[Abhiram Bindu Ramanathan](#) (Czech Technical University in Prague): Fracture and failure mechanism in molybdenum disulfide: Insights from molecular simulations

[Aneta Hrádková](#) (University of Chemistry and Technology, Prague): Structural variability of peptide deformylase

[David Bayer](#) (Brno University of Technology): MATLAB Interface To The afft Library

[Elliot Perviz](#) (Czech Technical University): Design rules for doped transition metal dichalcogenide heterostructures

[Gabriela Nečasová](#) (Brno University of Technology): Advancing PDE Solvers: A Taylor Series Approach

[Gowtham Nirmal Jonnalagadda](#) (University of South Bohemia in České Budějovice): Protein Junction Conductance – Cytochrome b562

[Hugo McGrath](#) (University of Chemistry and Technology, Prague): Gating of the Ribosome Exit Tunnel

[Ievgeniia Korniienko](#) (IT4Innovations): Terahertz spin-based sensors design

[Ivana Mihalikova](#) (Czech Academy of Sciences): Electronic structure calculations of GaAs using a quantum computer simulator

[Jakub Chlebík](#) (Brno University of Technology): Accelerating Ultrasound Treatment Planning with Gradient-Based Optimization Using JAX's Automatic Differentiation.

[Jakub Šebesta](#) (IT4Innovations): Magnetoelastic Properties of Pt-based systems

[Jan Zemen](#) (Czech Technical University in Prague): Analysis of magneto-optical Kerr spectra of ferrimagnetic Mn_4N

[Jiri Klimes](#) (Charles University): Testing the reliability of theoretical methods for predicting cohesive properties of molecular crystals

[Jiří Tomčala](#) (IT4Innovations): Face Gender Recognition Using Quantum Machine Learning on NVIDIA CUDA Quantum Simulator

[Jun Terasaki](#) (Czech Technical University in Prague): Neutrinoless double- β decay caused by Majorana neutrino

[Luigi Cigarini](#) (IT4Innovations): Effects of defected layers on the thermoelectric properties of scandium nitride thin films

[Marta Jaros and Ondřej Olšák](#) (Brno University of Technology): System for managing HPC-services and workflow executions

[Martin Mašek](#) (University of Chemistry and Technology, Prague): Exploring Ancestral Ribosome Models: Role of Protein Fragments and Evolutionary Significance

[Martin Melčák](#) (University of Chemistry and Technology, Prague): Molecular dynamics simulations of surface tension of hydrocarbon mixtures under high pressures

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- [Martin Niemczyk and Ondřej Vysocký](#) (IT4Innovations): Code continuous integration at IT4Innovations' systems
- [Michal Ďuriška](#) (Czech Academy of Sciences): Quantum-mechanical study of the electronic structure of diamond-structure crystals
- [Michal Svatoš](#) (Czech Academy of Sciences): Submission system for ATLAS jobs used on LUMI HPC
- [Miroslav Černý](#) (CEITEC, Brno University of Technology): Grain boundary segregation studied using machine-learned force fields
- [Oliver Kuník](#) (Brno University of Technology): Acceleration of hybrid local decomposition on Multi-GPU Systems
- [Ondřej Olšák](#) (Brno University of Technology): Investigating the Possibility of Using Pruned FFT in Ultrasound Wave Propagation Simulations
- [Pavel Papež](#) (Czech Academy of Sciences): Ab initio study of spin-polarization, atomic ordering and charge transfer in the CoCrNi medium-entropy alloy
- [Petr Sestak](#) (Brno University of Technology) and [Petr Sedlák](#) (Czech Academy of Sciences): AI based MD potential for NiTi shape memory alloy
- [Petr Touš](#) (University of Chemistry and Technology, Prague): Crystal structure prediction methodology for ionic liquids: In search of the unknown
- [Petra Čechová](#) (Czech Advanced Technology and Research Institute): From Fluidity to Rigidity: How Membrane Composition Influences Protein Conformation
- [Reynaldo II Geronia](#) (University of Chemistry and Technology, Prague): Comparing DFT-D3 and DFT-D4 models in predicting the thermodynamic properties of heterocyclic organic semiconductor crystals
- [Sergiu Arapan](#) (IT4Innovations): Calculating the Heisenberg exchange interactions via a supercell approach
- [Svitlana Pastukh](#) (Czech Academy of Sciences): In-Depth First-Principles Analysis of Structural, Electronic, Magnetic, and Lattice Dynamical Characteristics of $\text{Fe}_4(\text{P}_2\text{O}_7)_3$
- [Thibault Derrien](#) (IT4Innovations): Polaritonic qubit design and quantum computing for physics and chemistry
- [Valentína Berecová](#) (Czech Academy of Sciences): Quantum mechanical analysis of complex ferrimagnetic states in iron oxide nanoparticles