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 od Sciences): Electronic structure calculations of GaAs using a quantum computer simulator

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

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

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

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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 od Sciences): In-Depth First-Principles Analysis of Structural, Electronic, Magnetic, and Lattice Dynamical Characteristics of $Fe_4(P_2O_7)_3$

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

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