

7th Users' Conference of IT4Innovations

30–31 October 2023

[Alžběta Špádová](#) (ELI Beamlines): Nanoparticle Gas Target for Laser Wakefield Acceleration

[Antonio Cammarata](#) (Czech Technical University in Prague): Normal Dynamics: Solving Newton's Equations of Motion in the Reciprocal Space

[David Bayer](#) (Brno University of Technology): Acceleration of Heat Diffusion Simulation on Single-Node Systems

[Dominika Mášlarová](#) (Czech Academy of Sciences): Generation and Acceleration of Positrons by an Ultraintense Laser Pulse in a Plasma Channel

[Elliot Perviz](#) (Czech Technical University in Prague): Stabilisation of TMD-based Heterostructures for Tribological Applications

[Erik Andris](#) (Czech Academy of Sciences): Ab-initio Screening of Metal Binding Sites for Design of Small Metal-binding Peptides.

[Eugen Hruška](#) (Charles University): High-throughput Simulation of Protein Folding Dynamics

[Gabriela Nečasová](#) (Brno University of Technology): Parallel Numerical Solution of Differential Equations

[Gowtham Nirmal Jonnalagadda](#) (University of South Bohemia in České Budějovice): Quantum Transport in Protein Metal Junctions

[Ievgeniia Korniienko](#) (IT4Innovations): Theoretical Analysis of the Design of THz Radiation Spin-based Sensors and Their Potential Capabilities

[Indranil Saha](#) (Charles University): Exploring Proton Solvation and Water Diffusion in Acidic Zeolites: A Reactive Neural Network Approach for Aluminosilicate Systems

[Jakub Chlebík](#) (Brno University of Technology): Evolutionary Optimization of Architecture of an Ultrasound Propagation Neural Network Predictor

[Jan Ludík](#) (University of Chemistry and Technology): Hierarchy of Hydrogen Bonding among Bulk Liquid Hexanol Isomers

[Jemal Yimer Damte](#) (Czech Technical University in Prague): Designing a Material for a Photo-Triboelectric Nanogenerator in a Theoretical Perspective

[Jiří Tomčala](#) (IT4Innovations): Quantum Integer Factorization by Three Different Methods, Their Implementations and Results

[Jun Terasaki](#) (Czech Technical University in Prague): Reliability of Nuclear Matrix Element of Neutrinoless Double- β decay

[Marek Lampart](#) (IT4Innovations): iSOMA Swarm Intelligence Algorithm in Synthesis of Quantum Computing Circuits

[Martin Friák](#) (Czech Academy of Sciences): Structure-property Relations in Pb-supersaturated Metastable Sn-rich Pb-Sn Alloys

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Michael Owen (Masaryk University): The Mediation of Amyloid-beta Dimer Conformations by Gangliosides.

Michaela Černeková (University of Chemistry and Technology): Computer Simulations of the Early Moments of Peptide Synthesis

Michal Svatoš (Czech Academy of Sciences): Adapting the ATLAS Job Submission Systems to Changes in HPC Computing

Milan Kočí (Czech Technical University in Prague): Implementation of Particle Swarm Optimization algorithm into the programme FOX

Miroslav Černý (Brno University of Technology): Phosphorus Structures at the Copper (111) Surface

Mithun Manikandan (Czech Academy of Sciences): Structural Studies of Self-assembling Polymers

Ondřej Olšák a Marta Jaroš (Brno University of Technology): System for Managing HPC-services and Workflow Executions

Pavel Ondračka (Masaryk University): Machine-learning Potential for Amorphous WBC

Petr Chalupský (University of Chemistry and Technology): Conformational Dynamics of Model Peptides in Carbon Nanotubes

Petr Šesták (Brno University of Technology): Transferability of Machine-learned Force Fields for Different Types of Grain Boundaries

Petr Touš (University of Chemistry and Technology): Benchmarking Lattice Energies of Molecular Crystals: A Fragment-based ab initio Perspective

Petr Valenta (ELI Beamlines): High-power Laser Interaction with Gaseous Targets

Petra Svobodová (IT4Innovations): Developing New Methods for Securing Personal Documents

Prashant DWIVEDI (Czech Technical University in Prague): Unveiling the Mechanisms of Dust-Wall Interactions in Tokamaks: An Atomistic Study

Prokopis Hadjisolomou (ELI Beamlines): Gamma-Flash Via Multi-Petawatt Laser-Matter Interaction

Samuel Lukeš (Czech Academy of Sciences): First ERO2.0 simulations of Li & W redeposition on COMPASS Upgrade tokamak

Saurabh Kumar Pandey (Czech Academy of Sciences): Exploring Vibrational and Electromagnetic Properties of Protein Tubulin: A Computational Perspective

Sergiu Arapan (IT4Innovations): The Role of the Interface and Ferromagnetic Alloying on the Interlayer Exchange Coupling

Timothée Rivel (Masaryk University): Collective Variables for Evaluation of Pore Formation Energetics using Computer Simulations validated with Experimental Data