

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

4 – 5 November 2024

**10:00 – 11:00 | Registration and networking**

Monday, 4 November 2024

**11:00 – 11:30 | Welcome and IT4Innovations news**

**11:30 – 12:00 | KEYNOTE I**

*Chairperson: Martin Friák*

Synergy of semiempirical quantum chemistry and machine learning  
[Jan Řezáč | Czech Academy of Sciences](#)

**12:00 – 13:00 | Users' Talks I**

Machine learning assisted phonon calculations of Al-Ge solid solution  
[Martin Zelený | Brno University of Technology](#)

Introducing FireCore: Efficient Modeling Of (Small) Organic Molecules On Ionic Substrates  
[Paolo Nicolini | Czech Academy of Sciences](#)

Bottom-up machine learning potentials for peptides  
[Erik Andris | Czech Academy of Sciences](#)

**13:00 – 14:00 | Lunch & Poster Session**

**14:00 – 15:00 | Users' Talks II**

*Chairperson: Branislav Jansík*

Engineering Defect Clustering in Diamond-based Materials for Technological Applications via Quantum-mechanical Descriptors  
[Matúš Kaintz | Czech Technical University in Prague](#)

Efficient and accurate in silico polymorph ranking for molecular pharmaceuticals  
[Ctirad Cervinka | University of Chemistry and Technology Prague](#)

The Impact of Atomic Polarizability on the Thermodynamic and Structural Properties of Ionic Liquids  
[Martin Klajmon | University of Chemistry and Technology Prague](#)

**15:00 – 15:20 | Accessing EuroHPC Systems and Support from the High-Level Support Team (HLST)**

**15:20 – 16:20 | USERS' COUNCIL**

**16:20 – 16:50 | Coffee Break**

**16:50 – 17:20 | KEYNOTE II**

StreaMD: high-throughput automated molecular dynamics simulations tool  
[Pavel Polishchuk | Palacký University Olomouc](#)

**17:20 – 18:20 | Users' Talks III**

Structure and Tribological Properties of Mo-S-C Films via Reactive Molecular Dynamics  
[Iliia Ponomarev | Czech Technical University in Prague](#)

Multiscale modeling of magnetoelasticity  
[Dominik Legut | IT4Innovations](#)

Combined theoretical and experimental study of Fe-Sn intermetallic phases  
[Martin Friák | Czech Academy of Sciences](#)

**18:20 - 21:00 | Conference Dinner & Poster Session | 20:00 Tour of the IT4Innovations Data Room**

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**09:00 – 09:30 | KEYNOTE III**

Utilization of AI in Shape Optimization  
Michal Kravčenko | IT4Innovations

*Chairperson: Thibault Derrien*

**09:30 – 10:50 | Users' Talks IV**

Collimated  $\gamma$ -flash radiation via laser-target interaction  
Martin Matys | ELI Beamlines / Czech Technical University in Prague

State-Averaged Orbital-Optimized VQE: Enhancing Quantum Simulations for Ground and Excited States  
Silvie Illésová | IT4Innovations

“But it works on my machine” – escaping dependency hell through containerization for faster deployment in high-throughput docking benchmarks  
Dominik Suwala | Faculty of Pharmacy in Hradec Kralove, Charles University

Cratering of Tungsten Walls Under High-Velocity Dust Impacts  
Prashant Dwivedi | Czech Technical University in Prague

**10:50 – 11:20 | Coffee Break**

**11:20 – 12:20 | Users' Talks V**

Quasivalent Carbon: a new face-centred cubic carbon allotrope  
Antonio Cammarata | Czech Technical University in Prague

Interaction of Carbon Nanomaterials with Biomaterials  
Markéta Paloncýová | CATRIN, Palacký University Olomouc

Simulated nano-extrusion of graphene hyperbolic pseudosphere surfaces  
Peter Klaver | IT4Innovations

*Chairperson: Tomáš Kozubek*

**12:20 – 13:20 | Lunch**