

8th 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

Chairperson: Thibault Derrien

Utilization of AI in Shape Optimization
Michal Kravčenko | IT4Innovations

09:30 – 10:50 | Users' Talks IV

Collimated γ -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

Chairperson: Tomáš Kozubek

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

12:20 – 13:20 | Lunch