8th Users' Conference of IT4Innovations

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

4 – 5 November 2024

Monday 4 November 2024

10:00 – 11:00 | Registration and networking

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

11:30 – 12:00 | KEYNOTE I

Synergy of semiempirical quantum chemistry and machine learning
Jan Řezáč| Czech Academy of Sciences

12:00 – 13:00 | Users' Talks I   Chairperson: Martin Friák

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 – 16:10 | USERS' COUNCIL

16:10 – 16:40 | Coffee Break

16:40 – 17:10 | KEYNOTE II

StreaMD: high-throughput automated molecular dynamics simulations tool
Aleksandra Ivanova| Institute of Molecular and Translational Medicine

17:10 – 18:10 | Users' Talks III

Structure and Tribological Properties of Mo-S-C Films via Reactive Molecular Dynamics
Ilia 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

18:10 - 21:00 | Conference Dinner & Poster Session

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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