3RD USERS' CONFERENCE OF IT4INNOVATIONS

5-6 November

10:00 - 11:00 | Registration and networking

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

11:30 - 12:00 | KEYNOTE I

2D magnetic semiconductors - a power of HPC to predict
Dominik LEGUT | IT4Innovations

12:00 - 13:00 | Users' Talks I

Effects of liquid water on the stability and reactivity of zeolites
Andreas ERLEBACH | Charles University
HPC aspects of microscale urban climate modelling
Pavel KRC | Czech Academy of Sciences
Benzene radical anion in the context of the Birch reduction: when solvation is the key
Krystof BREZINA | Charles University
Modelling of lattice defects in advanced materials
Jana PAVLŮ | Masaryk University

13:00 - 14:00 | Lunch & Poster Session

14:00 - 15:30 | Users' Talks II

Theoretical study of effect of segregated impurities on the structure and properties of grain boundaries in Ni3Fe
Monika VŠIANSKÁ | Masaryk University
Accurate calculation of the binding strength of methane clathrate
Jiri KLIMES | Charles University
Alloy analogy model: Finite-temperature description of magnetic solids
David WAGENKNECHT | Charles University

14:45 - 15:30 | USERS' COUNCIL

15:30 - 16:00 | Coffee break

16:00 - 16:30 | KEYNOTE II

Ultrasound Simulation for Transcranial Neurostimulation
Jiri JAROS | Brno University of Technology

16:30 - 18:00 | Users' Talks III

Propene adsorption in alkali metal-exchanged FER zeolite
Miroslav RUBES | Czech Academy of Sciences
IT4I Satellite SAR Interferometry Monitoring System
Milan LAZECKY | IT4Innovations
Application of quantum-mechanical computational methods to computer-aided drug design
Jan ŘEZÁČ | Czech Academy of Sciences
Novel antiferromagnetic semimetal CuMnAs for spintronics applications
Karel CARVA | Charles University
Periodic DFT study of siting of divalent cations in silicon-rich zeolites
Stepan SKLENAK | J. Heyrovsky Institute of Physical Chemistry
Reaction Mechanism of Non-Heme Diiron Δ9-Desaturase: Why Does it Desaturate and Not Hydroxylate?
Lubomir RULISEK | Czech Academy of Sciences

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

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5-6 November

09:00 - 09:30 | KEYNOTE III

Double layer target with interface modulations for laser acceleration of collimated ion beams
Martin MATYS | Czech Technical University in Prague

09:30 - 10:30 | Users' Talks IV

Toward ab initio protein folding
Martin CULKA | Czech Academy of Sciences
Helium-based plasma interactions with air molecules
Martin BESEDA | IT4Innovations
How Do Atomistic Simulations of Huge Biomolecular Complexes Help Us Understand Protein Birth and Death?
Michal H. KOLAR | University of Chemistry and Technology
From gapped Goldstone to Higgs modes in excitonic magnets
Dominique GEFFROY| Masaryk University

10:30 - 10:45 | Coffee break

10:45 - 11:45 | Users' Talks V

Continuum and atomistic assessment of crack stability in nanocomponents
Petr ŠESTÁK | Brno University of Technology
Thermal conductivity of nuclear fuels from first principles
Lukáš KÝVALA | IT4Innovations
Nanoscale frictional properties of ordered and disordered molybdenum disulfide
Paolo NICOLINI | Czech Technical University in Prague
Rendering on an HPC cluster with R-a-a-S
Petr STRAKOS | IT4Innovations

11:45 - 13:00 | Lunch