Session Program

5–6 Nov 2026

10th Users' Conference of IT4Innovations

Poster Session

IT4Innovations, atrium
Studentská 6231/1B 708 00 Ostrava-Poruba

Thursday 5 November

17:30

Poster Session

Session | **Location:** IT4Innovations, atrium, Studentská 6231/1B 708 00 Ostrava-Poruba

17:30–17:31

From chemical ordering to mass transport: Machine-learning atomistic simulations of cubic TiAlON

Speaker
Pavel Ondračka

17:31–17:32

Effects of Hydrogen Occupation on the Magnetic and Electronic Properties of LaNi5- and LaNiSn-Based Hydrides: A DFT Study

Speaker
Kateřina Dočkalová

17:32–17:33

Use of open data for training machine-learning interatomic potentials

Speakers
Pavel Ondračka, Šimon Kratochvíl

17:33–17:34

Roofline Benchmarking and CPU-to-CPU Variability of Barbora NG

Speaker
Daniel Velicka

17:34–17:35

Modeling of High-Quality Electron Beam for a Compact EUV Free-Electron Laser

Speaker
Mihail Miceski

17:35–17:36

Multi-Level Compression for Direct Volume Rendering

Speaker
Markéta Faltýnková

17:36–17:37

Effective solution of differential equations on highly parralel architectures

Speaker
Petr Bém

17:37–17:38

Simulation Model of the Mitochondrial Ribosome

Speaker
Rudolf Kvasňovský

17:38–17:39

Anharmonic Effects in Tin Studied by MLIP

Speaker
Petr Sestak

17:39–17:40

Momentum-Resolved Energy-Loss Spectroscopy of Molybdenum Disulfide: First-Principles Interpretation of Experimental Spectra

Speaker
Michal Štulpa

17:40–17:41

Laser Wakefield Acceleration in Discharge-Generated Plasma Channels

Speaker
Alex Whitehead

17:41–17:42 **Radiation resistant refractory high entropy alloys**

Speaker
Mr Oussama Madyouni

17:42–17:43 **Blood Cell Membrane Models for Nanoparticle Delivery Systems**

Speaker
Petra Čechová

17:43–17:44

Hardware drift and the accuracy of molecular properties from quantum computers

Speaker
Przemyslaw Grenda

17:44–17:45 **Bringing Regional Traffic Simulation to HPC**

Speaker
Pavlína Smolková

17:45–17:46

First principles study of chalcogen vacancy effect on the optoelectronic and photocatalytic properties of transition metal dichalcogenides monolayers

Speaker
Tahir wahab

17:46–17:47

HPC-Enabled Real-Time Monitoring of Aseptic Gene Therapy Manufacturing Using Computer Vision

Speaker
Nikola Cudráková

17:47–17:48

A Comprehensive Stability Classification and Dynamical Analysis of a Brain-Inspired Coupled Rössler-Type System

Speaker
Haseeba Sajjad

17:48–17:49

Biased-exchange metadynamics of nascent peptide-accompanied rearrangements of the ribosome catalytic center

Speaker
Josef Cikhart

17:49–17:50

Tuning magnitude and direction of lattice thermal conductivity in transition metal dichalcogenide heterobilayers

Speaker
Mr Elliot Perviz

17:50–17:51

Case study: Six months of work from heat flow simulation to the arrow of time experiment.

Speaker
Ladislav Ničman

17:51–17:52

Privacy-preserving federated learning with light-weight attention improved CNNs for automated leukemia detection across distributed medical imaging

Speaker
Muhammad Zeerak Awan

17:52–17:53

Influence of the N/P ratio on Lipid Nanoparticle's structure and behaviour

Speaker
Adéla Chadalíková

17:53–17:54

Polypyridine Iron Complexes in Elektro- & Photocatalytic CO2 Reduction

Speaker
Florian Lemken

17:54–17:55

Regional climate projections of non-CO2 forcers and their impact on climate and air quality using RegCM5-Chem

Speaker
Natália Machado Crespo

17:55–17:56

Predicting polymorphs of pharmaceutical co-crystals via crystal structure prediction

Speaker
Petr Touš

17:56–17:57

Spectroscopy Enhanced by Two-Dimensional Materials for the Detection of Free Heme Associated with Intravascular Hemolysis

Speaker
Angarag Munkhbat

17:57–17:58

Thermoelectric properties of defective scandium nitride nanostructures from first principles

Speaker
Luigi Cigarini

17:58–17:59

Machine Learning for Predicting Lignin Solubility and Guiding Solvent Selection

Speaker
Zaheer Abbas

17:59–18:00

Effects of sequence on the conformational ensembles of ribosomal protein fragments

Speaker
Jan Heblt

18:00–18:01

Atom-scale contributions to nanofriction response in transition metal dichalcogenides

Speaker
Mr Suresh Ravisankar

18:01–18:02

A Quantum Perspective on Interval Power Flow

Speaker
Michal Belina

18:02–18:03

Density functional theory simulations of hydrogenated graphene supported by machine learning

Speaker
Jiří Richter

18:03–18:04

Many-body errors of quantum chemistry methods

Speaker
Jiri Klimes

18:04–18:05

Energy-optimized scaling laws for laser-driven electron accelerators

Speaker
Dr Petr Valenta

18:05–18:06

From Batch Jobs to AI Services: Training and Inference Workflows on HPC

Speaker
Tomáš Martinovič

18:06–18:07

Quantum-Circuit Tensor Networks for Correlated Superconducting Nanostructures

Speaker
Jan Hojač

18:07–18:08

SELECTING VAN DER WAALS FUNCTIONALS FOR 2D MAGNETS: A DFT BENCHMARK FOR STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF CHROMIUM TRIHALIDES (CrX_3)

Speaker
SUBHASMITA RAY

18:08–18:09

Kinetic study of shock formation in protostellar jets

Speaker
Jakub Gazdoš

18:09–18:10 **Influence of Antisite Defects on the Stability of Martensitic NiTi**

Speaker
Petr Jaroš

18:10–18:11
Evaluating Generative Structural Models Against Multi-Microsecond Molecular Dynamics for Intrinsically Disordered Ensembles: Lessons from p53 TAD1

Speaker
Michael Bakker

18:11–18:12
Laser-driven acceleration of sub-GeV and GeV high-quality electron beams

Speaker
Dr Martin Matys

18:12–18:13
Atomistic Insights Into Interaction of Doxorubicin With DNA: From Duplex to Nucleosome

Speaker
Andrea Nedělníková

18:13–18:14
Controlled Electron Injection and keV Betatron X-rays from Nanoparticle-Assisted Laser Wakefield Acceleration

Speaker
Alfred Mishi

18:14–18:15
Magnetic field effect on acoustic wave propagation in cubic ferromagnets

Speaker
Ievgeniia Korniienko

18:15–18:16
Machine-learned interatomic potentials for fracture simulations in hydroxylated silica minerals

Speaker
Valentína Berecová

18:16–18:17 **Simulation-Driven Optimization of Betatron X-ray Sources**

Speaker
Dominik Čáp

18:17–18:18
The stability and material properties of Zn5Sb4In2 computed by quantum mechanical calculations

Speaker
Martin Friák

18:18–18:19 **Implicit solvation models for modern neural network potentials**

Speaker
Erik Andris

18:19–18:20
The Quantum Access Trail: Reach QPUs at EU/National scale with QHEAppE

Speaker
Jan Swiatkowski

18:20–18:21
Developing Machine Learning Interatomic Potential for 2D TMDC High Entropy Alloys

Speaker
Shubham Agarwal

18:21–18:22 **Magnetoelastic behavior in tetragonal Pt-base compounds**

Speaker
Dr Jakub Šebesta

18:22–18:23
Interlayer exchange coupling in antiferromagnetic multilayers with magnetically alloyed spacer

Speaker
Sergiu Arapan

18:23–18:24
Bridging Phonon Dynamics and Nanotribology in TMD Heterostructures via Machine Learning Force Fields

Speaker
Ravikant Kumar

18:24–18:25
Feature-Complete Multi-GPU Solver for the k-Wave Ultrasound Simulation Toolbox

Speaker
Oliver Kuník

18:25–18:26
Modular multiscale approach to modelling HHG in gases & spectrally selective HHG scheme

Speaker
Jan Vábek

18:30