9th Users' Conference of IT4Innovations

Thursday, 30 October 2025

Conference Dinner and Poster Session - atrium (18:20 - 21:00)

time	[id] title	presenter
18:20	[275] Suitable boron-doped graphene substrate for glucose Raman signal enhancement	CAMMARATA, Antonio
18:21	[265] New potential for atomistic simulations in NiTi martensite	ŘEHÁK, Petr
18:22	[306] Characterizing Nonlinear Dynamical System Behaviors Using Self-Organizing Maps with Clustering Techniques	Ms EHSAN, Haiqa AWAN, Muhammad Zeerak
18:23	[305] On the role of point defects and metal clustering in the mechanical properties of titanium aluminium oxynitride coatings	ONDRAČKA, Pavel
18:24	[270] Membrane selectivity of Opi1 peptide derivatives	HERNÁNDEZ TANGUMA, Alejandro
18:25	[292] Atomistic Insights into the Structure and Dynamics of Lipid Nanoparticles	CHADALÍKOVÁ, Adéla
18:26	[256] Running a mixture of ATLAS jobs with widely ranging resource requirements at IT4Innovation	SVATOŠ, Michal
18:27	[271] Benchmarking GW Methods for Accurate Prediction of Defect States in Doped Diamond	KAINTZ, Matúš
18:28	[282] Analysis of Magnetic Spin Disorder in Ferrimagnetic Iron Oxides with DFT and Beyond-DFT Approaches	BERECOVÁ, Valentína
18:29	[293] Benchmarks of composite quasi-harmonic models of polymorphism in benzophenone and sulfamerazine	GERONIA, Reynaldo II
18:30	[300] EasyDock 1.0: customizable and scalable docking tool	Ms MINIBAEVA, Guzel
18:31	[287] Optimisation of k-Wave Ultrasound Wave Propagation Simulations Through Fourier Transform Pruning	OLŠÁK, Ondřej
18:32	[273] Deep Potential Molecular Dynamics Study of Au(111)/MX2/Si tip	Mr RAVISANKAR, Suresh
18:33	[284] Quantum-mechanical analysis of H7LaNi5-xSnx	DOČKALOVÁ, Kateřina
18:34	[307] A Scalable Framework with Modified Loop-Based Multi-Initial Simulation and Numerical Algorithm for Classifying Brain-Inspired Nonlinear Dynamics with Stability Analysis	SAJJAD, Haseeba
18:35	[302] The magnetic exchange coupling in Co/Ru/Co trilayers: a study of the bilinear and biquadratic coupling parameters by electronic structure calculations.	ARAPAN, Sergiu
18:36	[278] Developing Machine Learning Force Fields for Transition Metal Dichalcogenides with metallic substrate Ag and Si AFM tip	Dr CAMMARATA, Antonio KUMAR, Ravikant
18:37	[286] Light Utilization for Matter Emergence	VÁBEK, Jan
18:38	[304] Use of open data for training machine-learning interatomic potentials	KRATOCHVÍL, Šimon
18:40	[257] Response of twins in NiTi martensite to mechanical loading	ČERNÝ, Miroslav
18:41	[279] Molecular Dynamics Refinement of Cytochrome P450 Docked Complexes	GRENDA, Przemyslaw
18:42	[288] Conformational preferences of ribosomal protein fragments	HEBLT, Jan

18:43	[290] Local vs. Global FFT Approaches for High-Performance Ultrasound Simulation on Multi-GPU Systems	KUNÍK, Oliver
18:44	[266] The role of non-canonical amino acids on the protoribosome	KŘIVAN, Michael
18:45	[294] Optimizing NiTi Interatomic Potentials Through Atomic Cluster Expansion	SESTAK, Petr
18:46	[272] Tuning the atomic scale friction of doped transition metal dichalcogenides heterostructures: First steps	Mr PERVIZ, Elliot
18:47	[267] Preliminary ERO2.0 erosion and transport simulations of tungsten impurities for COMPASS Upgrade	LUKEŠ, Samuel
18:48	[261] Spin-lattice model for computational study of elastic response to ultrafast demagnetization in fcc Ni	KORNIIENKO, Ievgeniia
18:49	[285] Modular Multiscale Approach (MMA) to simulate high harmonic generation in gases and applications	VÁBEK, Jan
18:50	[299] Gating of the ribosomal exit tunnel	MCGRATH, Hugo
18:51	[274] Magnetoelastic Properties in MnPt magnetic systems	Dr ŠEBESTA, Jakub
18:52	[303] Machine Learning Based Interatomic Potential for Martensitic NiTi	JAROŠ, Petr
18:53	[258] ElaStr: An Online Tool Linking Elastic Properties and Crystal Structures	ZELENÝ, Martin
18:54	[291] Numerical study of oscillations in solar prominence threads excited by vortex shedding	Ms BELOV, Sofya
18:55	[277] The role of emissions in future Central European air-quality scenarios	PRIETO PEREZ, Alvaro Patricio