Posters

Alaukik Saxena
A materials informatics framework to discover patterns in atom probe tomography data
Alena Vishina
High-throughput and Data-mining Search for Rare-earth-free Permanent Magnets
Alfonso Gallo Bueno
Unsupervised machine learning for detection of spurious structures
Amirhossein Naghdi Dorabati
Mechanical properties of crystalline W and Mo metals by Neural network interatomic potentials
Andreas Møller Slavensky
Searches for stable nano-sized silicates clusters in the interstellar medium
Antti Pihlajamäki
Orientation Adaptive Minimal Learning Machine for Atomic Forces
Avula Venkata Siva Nikhil
Prediction of Shear Viscosity of Complex Fluids Using Machine Learning Methods: Model Performance, Ranking, Interpolation, and Uncertainty Quantification
Carlo Maino
Excited State Machine Learning for Chromophores in Complex Environments
Cesare Malosso
Viscosity in water from first-principles and deep-neural-network simulations
Claudio Zeni
Exploring the robust extrapolation of high-dimensional machine learning potentials
Connor Allen
A Computationally Efficient Approach for Improving Phonon Representation in Machine Learned Potentials
Fabio Priante
Identifying Unknown Organic Molecules in Atomic Force Microscopy Images through Deep Generative Models
Hannes Kneiding
Machine Learning Quantum Properties of Transition Metal Complexes using Graph Neural Networks
Hyunwook Jung
Global optimization protocol for adsorbate geometries using an on-the-fly surrogate Gaussian Approximation Potential
Ibrahim Buba Garba
Temperature-dependent phonons from ab-initio simulations
Indranil Saha
Understanding Germanosilicate Hydrolytic (In)stability based on Germanium Distributions derived using Neural Network Potentials
Iuri Macocco
An intrinsic dimension estimator for discrete-metric spaces
Jean Baptiste Fankam
Theoretical investigation of the molecular structure, vibrational spectra, thermodynamic and nonlinear optical properties of 4, 5-dibromo-2, 7dinitro- fluorescein
Johannes Döhn
Computational Screening of Oxide Perovskites as Insertion Type Cathode Materials
Kevin Rossi
Data-driven modelling and characterization of Au nanoparticles melting
Khatereh Azizi
Unsupervised learning on solvation of molecules in water

Kunal Ghosh
Assessing the potential of active machine learning for curating molecular datasets
Kushal Ramakrishna
Physics-informed and data-driven molecular dynamics simulations of Iron under extreme conditions
Kyeonghyeon Nam
Ab Initio Thermodynamics for Surface Motifs of the M1 Selective Oxidation Catalyst
Lakshmi Shenoy
Developing a machine learning interatomic potential for simulation of fracture in irradiated *alpha*-iron
Lars Leon Schaaf
Machine Learned Force Field for Oxides as Catalysts
Lauri Kurki
A scanning probe microscopy study into the hydration of an adenine self-assembled monolayer
Lea Gašparič
Towards predicting corrosion inhibitors' performance with machine learning
Lei Zhang
Active Learning of Gaussian Approximation Potential: Application for Fracture in Iron
Lucas Lang
Δ-Machine Learning with Equivariant Graph Neural Networks
Mahmoud Attia
Multiscale Modeling of lithium diffusion and NMR properties in ceramics solid electrolytes for the new generation of solid state batteries
Mandana Safari
Correct Vibrational Properties of Polar Materials from Neural Network Interatomic Potentials
Mani Lokamani
Evolution of Single-Level-Model parameters in the Mechanically controllable Break Junctions
Manuel Kuchelmeister
Multi-fidelity machine learning to accelerate materials research
Marco Bertolini
Unsupervised Learning of Group Invariant and Equivariant Representations
Mohsen Sotoudeh
Understanding ion mobility mechanism through the descriptor and scaling relations in solid crystallines
Nikolaj Rønne
Global atomistic optimisation enhanced by local surrogate model
Nejc Hodnik
Using Machine Learning to Predict Activity from Synthesis Parameters for PtCu Alloy Fuel Cell Nanoparticulate Electrocatalysts
Niko Oinonen
Molecule graph reconstruction from Atomic Force Microscopy images with machine learning
Nore Stolte
Reactions of aqueous carbon at deep Earth pressure and temperature conditions
Ondrej Krejci
Density Functional Theory models simulating Kelvin Probe Force Microscopy with flexible tip apices
Pablo Sánchez-Palencia Vallejo
Exploring the configurational space of spinel phase (Sn1-xGex)3N4 solid solutions with machine learning
Riccardo Dal Molin
Development a DeePMD potential for monolayer WTe2
Romina Wild
Identifying informative distance measures in high dimensional feature spaces: Application to COVID-19 severity prediction

Ruggero Lot
PANNA: a comprehensive toolkit for creating neural network models for atomistic systems
Samare Rostami
Exploring the novel mixed TiO2/ZrO2 structures and interfaces from structure predictions based on charge equilibration via neural network technique.
Sebastian Havens
Investigation of the phase behaviour of embedded atom models of metals using nested sampling and coexistence simulations
Simone Di Cataldo
Mapping Superconductivity in High-Pressure Hydrides
Uroš Hribar
Modeling the relation between processing parameters and material properties in foamed glass production with machine learning
Valerio Briganti
Extending spectral neighbour analysis potentials with long range physics
Wojciech Stark
Investigation of nonadiabatic effects for H2 at Cu surfaces: A unified machine-learned electronic friction model for multiple facets
Xi Chen
Baysian Optimization Conformer Search of Molecular Adsorbates on a Gold-thiolate Cluster
Yonghyuk Lee
Ab Initio Thermodynamics for Surface Motifs of the M1 Selective Oxidation Catalyst
Yuxuan Yao
Modified active machine learning (AML) approach to explore the molecular design through the use of surrogate models for charge injection and transport descriptors.