Vladimir Ladygin

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Computational materials scientist

MLIPs| DFT & Classical simulation | Deep learning | AI for materials design

As a materials researcher with a focus on computational modeling, I specialize in leveraging advanced computational techniques to study and understand the properties of materials. My expertise spans various fields including AI-guided material design, machine learning interatomic potentials (MLIP) developments, large-scale molecular dynamics, and ab initio simulations and HPC programming. With strong analytical and communication skills, I excel in translating complex scientific requirements into technical specifications and designing functional process architectures for materials research.

WORK EXPERIENCE

California Institute of Technology - *Pasadena, California* 09/2020 – 06/2024

Graduate Researcher

Performed materials characterization with inelastic neutron scattering technique complemented by ab initio and classical molecular dynamics simulations and scientific programming on C/C++ and Python

- performed modern inelastic neutron scattering experiments followed by analyses of multidimensional datasets on Python;
- designed HPC pipelines for the automatic calculation of thermodynamics properties using machine learning interatomic potentials, optimizing computing and communication time of control scripts, ab initio (VASP) and classical MD (LAMMPS) codes, and AI models;
- developed software for accelerated computations of materials' vibrational properties using MPI and GPU parallelization coming from molecular dynamics simulation in HDF5 file format, resulting in a 50% computing time reduction for the MPI version and a 99% time reduction for GPU implementation;
- designed scientific experiments, completing more than 10 projects over 4 years;
- as an expert in scientific computing in the group managed computational directions of the projects, providing guidance and mentorship to younger researchers;
- optimized, trained and build machine learning interatomic potentials for solid matter systems
- studied electron-phonon interaction in semiconductors using advanced first principles software (QE, EPW)
- designed analytical models explaining fundamental materials behavior, gave conferences talks, and lectures, participated in multiple publications;

Skolkovo Institute of Technology - *Moscow, Russia* 09/2018 – 01/2021

Junior Researcher | Scientific Computing

Developed AI-based software for free energy and phase diagram calculation from statistical thermodynamics data obtained

in molecular dynamics simulations using numerical libraries in C/C++ and Python

- designed Gaussian Process-based methodology for automatic estimation of free energy and construction phase diagrams of materials with confidence intervals 10 times reducing the requirement on dataset size compared to traditional methods;
- implemented HPC pipeline to automate the process of thermodynamical data collection required for the training set construction and active learning;
- extended capabilities of Python numerical libraries with C++ extensions for long-range arithmetic reducing the computational time by 90%;
- extended capabilities of the software with tensor decomposition-based Bayesian neural networks allowing high dimensional data utilization
- guided and trained team members on HPC computing, improving team performance and knowledge sharing.

All-Russia Institute of Automatics named by Duhov - *Moscow, Russia* 09/2017 – 01/2021

Junior Researcher | Computational Materials Scientist

Performed machine learning potential training and large-scale simulation of materials mechanical properties.

- 3+ years of experience in HPC computing, python programming, bash scripting and Linux systems
- assisted in developing and writing proposals;
- designed and developed complex HPC pipelines (calculations, io, postprocessing) resulting in improved accuracy and efficiency of molecular dynamics and ab initio simulations;
- trained ab initio level accuracy machine learning-powered models for more than 10 physical systems;
- tuned active learning procedures resulting in a total dataset reduction of 25%;
- performed simulation of vibrational and mechanical properties of materials using statistical analysis techniques

HZDR - *Dresden, Germany* 06/2018 – 09/2018

Computational Materials Scientist (Internship)

Performed large-scale molecular dynamics simulation of two-dimensional materials under ion clusters irradiation.

- implemented HPC calculation pipeline for the Molecular Dynamics study of MoS_2 2D material under irradiation with noble gases, my workflow allowed an efficient collection and postprocessing of simulation data with multiple ion types, collision angles, and impact sites of noble gases clusters;
- developed an unsupervised learning algorithm with >90% accuracy of ion sputtering clusterization;
- made a significant contribution to the study resulting in a future publication in high impact journal.

DESY - *Hamburg, Germany* 06/2017 – 09/2017

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Computational Physicist (Internship)

MATLAB programming for analysis of large datasets on 3D X-ray imaging coming from Deutsch Electron Synchrotron

- analyzed multidimensional datasets using software written in MATLAB for analytical models and real experiments;
- documented and tested over 100 scenarios of GaN nanowire deformation improving the accuracy of X-ray imaging phase retrieval by 15%;
- successfully managed a remote full-time job internship and university applications at the same time.

EDUCATION

California Institute of Technology – *Pasadena, CA*

Doctor of Philosophy – Applied Physics and Materials Science, 2020 – 2024

California Institute of Technology – *Pasadena, CA*

Master of Science – Applied Physics and Materials Science, 2020 – 2022

Skolkovo Institute of Science and Technology – *Moscow, Russia*

Master of Science – Computational Materials Science, 2018 - 2020

Moscow Institute of Physics and Technology - *Moscow, Russia*

Master of Science – Applied Physics and Mathematics, 2018 – 2020

Moscow Institute of Physics and Technology - *Moscow, Russia*

Bachelor of Science – Applied Physics and Mathematics, 2014 – 2018

Publications

[1] Ladygin, V., Korotaev, P., Yanilkin, A., Shapeev, A. (2020). Lattice dynamics simulation using machine learning interatomic potentials. Computational Materials Science, 172, 109333.

[2] Ghaderzadeh, S., Ladygin, V., Ghorbani-Asl, M., Hlawacek, G., Schleberger, M., Krasheninnikov, A. (2020). Freestanding and Supported MoS2 Monolayers under Cluster Irradiation: Insights from Molecular Dynamics Simulations. ACS Applied Materials and Interfaces, 12(33), 37454-37463.

[3] Ladygin V., Beniya I., Makarov E., and Shapeev A. (2021). Bayesian learning of thermodynamic integration and numerical convergence for accurate phase diagrams. Physical Review B 104, 104102.

[4] Miryashkin, T., Klimanova, O., Ladygin, V., & Shapeev, A. (2023). Bayesian inference of composition-dependent phase diagrams. Physical Review B, 108(17), 174103.

PROFESSIONAL SKILLS

- DFT codes: VASP, QE, gaussian
- MLIPs
- Molecular dynamics codes: LAMMPS, GROMACS
- Phonon calculations: Phonopy, TDEP, dynasor
- TensorTrain learning
- Machine learning engineering
- Deep learning
- Bayesian analyses
- C/C++, Python
- Deep Bayesian learning
- High-performance computing
- GPU programming
- Software development