Daniil Alekseev

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Summary

Aspiring computational materials science researcher with a strong foundation in Applied Mathematics and Physics. Focused on leveraging Molecular Dynamics (MD) and Density Functional Theory (DFT) methods, augmented by an expertise in developing and applying machine learning interatomic potentials and other applications of Machine Learning, to investigate complex material properties.

Education

Skolkovo Institute of Science and Technology (Skoltech) *2025-2027* (expected)
MSc in Materials Science

Moscow institute of physics and technology (MIPT) *2021-2025*
BSc in Applied Mathematics and Physics, Landau Phystech School of Physics and Research
GPA: 4.65/5.00 (7.7/10.0)
Additional Professional Education: Advanced Machine Learning Methods (2024)

Research Expertise

Computational Materials Design Laboratory, MIPT *March 2024 – current time*
Bachelor Thesis: Excitation Spectra in Liquid Carbon using ML Potentials

- Investigated anomalous sound velocity behavior in liquid carbon at high temperatures (>5000K) to explain experimental phenomena.
- Trained and deployed Moment Tensor Potentials (MLIP) from scratch using data generated from DFT (VASP) calculations.
- Performed large-scale MD simulations (LAMMPS) to calculate structural and acoustic properties, successfully linking density decrease to sound velocity increase.
- **Outcome**: Authored a bachelor's thesis and presented key findings at multiple scientific conferences. Publication in preparation.

Laboratory of Multiscale Modeling *January 2023 – December 2023*
in Soft Matter Physics, MIPT
Thermodynamic and Mechanical Properties of Monolayer Fullerene Networks

- Applied the pre-trained GAP-20 machine-learning potential within the LAMMPS framework on supercomputer clusters to enable simulations for novel quasi-tetragonal fullerene (C60) networks.
- **Outcome**: Co-authored a scientific article in *Computational Materials Science* and presented results at the 65th MIPT All-Russian Scientific Conference.

Center of NTI "Digital Materials Science", BMSTU
Laboratory Technician *March 2025 – current time*
Automated Polymer Potential Generator

- Currently developing an open-source Python package to create a data-driven workflow for automatically training interatomic potentials for polymer simulations.
- The tool aims to bridge DFT accuracy with MD efficiency for polymer property prediction. (Link to GitHub)

Core Skills

Computational Methods: Molecular Dynamics (MD), Density Functional Theory (DFT), Quantum Chemistry, Monte Carlo **Simulation Packages:** LAMMPS, VASP, Quantum Espresso, PySCF **Programming & Data Science:** Python (PyTorch, TensorFlow, Pandas, Scikit-learn), C++, Bash Scripting, HPC computations **Physics Expertise:** Solid State Physics, Statistical Physics, Condensed Matter Theory

Publications & Presentations

1. Алексеев Д. С., Орехов Н. Д. Расчет механических и теплофизических свойств кристаллического монослоя фуллеренов С60 методом молекулярной динамики // Труды 65-й Всероссийской научной конференции МФТИ в честь 115-летия Л.Д. Ландау, 3–8 апреля 2023 г. Электроника, фотоника и молекулярная физика. М.: Физматкнига, 2023. С. 48-49.

2. Алексеев Д. С., Орехов Н. Д. Расчет спектра возмущений для жидкого углерода методами классической молекулярной динамики с машинно-обучаемыми потенциалами // Материалы 67-й Всероссийской научной конференции МФТИ, 30 марта–5 апреля 2025 г. Фундаментальная и прикладная физика: С. 459-462.

3. Alekseev, D., Logunov, M., Lazarev, M., Zhukov, S., & Orekhov, N. (2025). Thermal stability of monolayer fullerene networks: A molecular dynamics study with machine-learning potential. Computational Materials Science, 248, 113572. https://doi.org/10.1016/j.commatsci.2024.113572

Achievements

- Lead a six people team in a month-long hackathon held among students of the course of additional professional education "Advanced Machine Learning Methods".
- Participated in an accelerator for student projects at Skoltech in a multidisciplinary team of five people finishing in third place in "Materials & Devices" cohort

Languages

Russian: Native
English: Upper Intermediate (B2+)
Chinese: Elementary (A2+/HSK3)