YULIA PIMONOVA

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PROFESSIONAL SUMMARY

Computational chemist and machine learning researcher with 6+ years developing scalable ML frameworks and high-performance simulation pipelines for molecular science. Expert in Python, PyTorch, and scientific computing with proven success deploying meta-learning algorithms, cheminformatics tools, and open-source packages. Track record of securing funding, mentoring cross-functional teams, and publishing in top-tier journals (JACS, 11 publications, h-index: 7).

TECHNICAL SKILLS

Programming & ML: Python (advanced), PyTorch, Scikit-learn, XGBoost, Graph Neural Networks, MAML, Meta-Learning
Scientific Computing: NumPy, SciPy, Pandas, Matplotlib, HOOMD-blue, LAMMPS, Molecular Dynamics, DFT
Tools & Infrastructure: Git, CI/CD, SLURM, HPC, Linux/Unix, Jupyter, LaTeX, AWS basics, Open-source development

PROFESSIONAL EXPERIENCE

Postdoctoral Research Associate May 2024 – Present
Los Alamos National Laboratory *Los Alamos, NM*

- Developed meta-learning framework for molecular property prediction achieving superior small-data performance; methodology adopted across 3 LANL divisions (bio, environmental, seismology); paper under review at *Nature Machine Intelligence*
- Built open-source Python package (**buhito**) for graphlet analysis, implementing optimized DFS/BFS algorithms; secured $500K+ funding as sole postdoc on multi-PI computational chemistry project
- Contributed core cheminformatics functionality to **minervachem** library for SeparationML project, developing automated filtering pipelines and substructure visualization tools for metal-metal separation ligand design
- Mentored 2 graduate students (Statistics, CS backgrounds) in 2025 with 100% project acceptance rate at Applied ML Summer School; expanding to 3 mentees in 2026
- Organized Telluride Workshop on ML for Chemistry (40+ participants), managing invitations, scheduling, and facilitating discussions; received outstanding feedback on pre-workshop survey methodology

Graduate Research Assistant, PhD Student May 2020 – May 2024
University of Utah, Department of Chemistry *Salt Lake City, UT*

- Engineered custom MD simulation pipeline processing 500K+ particle cocrystallization systems on GPU-accelerated HPC clusters using HOOMD-blue; generated 10+ TB datasets for ML analysis
- Published first-author paper in *J. Am. Chem. Soc.* (JACS) demonstrating thermodynamic stability is poor predictor of cocrystal formation, challenging pharmaceutical industry conventional approaches
- Automated analysis workflows combining NumPy, Pandas, and Freud to extract thermodynamic/kinetic parameters from terabyte-scale simulation data, reducing analysis time by 70%
- Developed OOP Python packages for molecular visualization adopted by 5+ lab members, reducing code duplication by 50%

EDUCATION

PhD in Physical Chemistry, GPA: 3.98/4.0 (Summa Cum Laude) Aug 2019 – May 2024
University of Utah *Salt Lake City, UT*

B.Sc. in Chemistry, GPA: 4.0/4.0 (Summa Cum Laude) Sep 2014 – Jun 2019
Southern Federal University *Rostov-on-Don, Russia*

SELECTED PUBLICATIONS & IMPACT

11 Publications (3 First-Author, 3 arXiv Preprints) | H-index: 7 | 150+ Citations

- **Pimonova, Y.**, et al. "Meta-Learning Linear Models for Molecular Property Prediction." *arXiv:2509.13527*, 2025.
- **Pimonova, Y.**, Carpenter, J.E., Gruenwald, M. "Thermodynamic Stability Is a Poor Indicator of Cocrystallization." *J. Am. Chem. Soc.*, 2024, 146(4), 2815-2824. (24 citations)
- Datta, S., et al. (incl. **Pimonova, Y.**) "Statistical Insight into Meta-Learning via Predictor Subspace." *arXiv:2509.18349*, 2026.

AWARDS & LEADERSHIP

Selected Awards: Team Distinguished Award (LANL, 2025), Poster Prize (Berkeley Stat Mech Meeting, 2023), Best Teaching Assistant (U. Utah, 2020), Amgen Women in Chemistry Fellowship (2023)
Leadership: Organizer, Telluride ML Workshop (2025); AML Summer School Mentor (2025-26); Coordinator, Graduate Research Symposium (2023); Discussion Leader, Gordon Research Seminar (2023)