YULIA PIMONOVA

Santa Fe, NM | U.S. Permanent Resident (Green Card) | Open to relocation | Open to remote
pimonova.ya@gmail.com | Personal Website | LinkedIn | GitHub | Google Scholar

PROFESSIONAL SUMMARY

Computational chemist with 6+ years of experience spanning molecular dynamics, scientific computing, ML/AI for science, and HPC. Expert in leveraging Python and ML frameworks to solve complex problems in molecular property prediction. Track record of developing scalable algorithms and optimized workflows for research applications. Experienced in scientific program management and workshop organization, including agenda design, speaker coordination, logistics, and execution. With 3+ years of experience in materials synthesis and characterization, I can lead full-stack chemical R&D and efficiently navigate cross-team projects.

DOMAIN EXPERTISE: Chemistry and Materials, Molecular Dynamics, Graph Theory, Meta-Learning

TECHNICAL SKILLS

Scientific Computing: Python, NumPy, SciPy, Pandas, Matplotlib, Seaborn, ASE, RDKit, NetworkX, Dask
Coding: Shell, Data Visualization, Git, Slurm, HPC, Linux, Jupyter, Unit testing, Code optimization
ML & AI: PyTorch, Scikit-learn, XGBoost, Graph Neural Networks (GNN), Deep Learning, Reinforcement Learning, Active Learning
Computational Chemistry: Molecular Dynamics (MD), Density Functional Theory (DFT), Gaussian, Q-Chem, LAMMPS, HOOMD-blue
Data Management: Notion, Obsidian, LaTeX, Markdown

PROFESSIONAL EXPERIENCE

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

- Developed meta-learning framework for molecular property prediction, achieving up to 25x accuracy improvement in small-data regimes; paper under review and methodology adopted by bio, environmental, and seismological divisions across LANL
- Building open-source Python package buhito for graphlet analysis on molecular graphs (public release pending approval), implementing DFS and BFS algorithms with comprehensive benchmarking suite; secured funding as postdoc Co-I
- Contributed core functionality to minervachem cheminformatics library for SeparationML project, developing automated filtering pipelines, substructure visualization tools, and data parsing capabilities to accelerate ligand design for metal-metal separations
- Designed and secured funding for 3 summer research projects for Applied Machine Learning Summer School with 100% acceptance rate; mentored 2 graduate students (Statistics, Computer Science backgrounds) in 2025, expanding to 3 mentees in 2026
- Organized and led Telluride Science Workshop on Machine Learning and Informatics for Chemistry and Materials (2025), managing invitations, scheduling, and facilitation of 40+ participants; designed pre-workshop survey driving highly-rated group discussions on the state of ML in science
- Applied Model-Agnostic Meta-Learning (MAML) and linear meta-learning techniques to predict chemical properties of PFAS molecules, enabling rapid model adaptation across diverse environmental contamination scenarios
- Co-authored 2 competitive proposals for LANL funding opportunities, designing strategies and technical visualizations for ML-driven coarse-graining and graph-theoretic analysis projects, with the graph project being funded

Summer Research Intern June 2023 – August 2023

Los Alamos National Laboratory, mentored by Dr. Nicholas Lubbers *Los Alamos, NM*

– Adopted meta-learning paradigm to linear models in chemistry for the first time
– Developed a custom meta-learning algorithm for linear models based on the common subspace assumption, tested on small (< 3000 datapoints) and moderate (134k) datasets, both experimental and computational data
– Onboarded as developer on minervachem cheminformatics Python package, resolved critical bugs

Graduate Research Assistant May 2020 – May 2024

University of Utah, Department of Chemistry (Prof. Michael Gruenwald Group) *Salt Lake City, UT*

– Advanced cocrystallization theory by establishing that thermodynamic stability is a poor predictor of cocrystal formation, challenging conventional approaches and informing new prediction methodologies for pharmaceutical applications
– Designed and developed custom molecular dynamics simulation pipelines for large-scale cocrystallization studies, processing 500K+ particle systems using HOOMD-blue on GPU-accelerated HPC clusters
– Engineered automated analysis workflows in Python combining NumPy, Pandas, and Freud to extract thermodynamic and kinetic parameters from terabytes of simulation data, reducing analysis time by 70%
– Developed object-oriented Python packages for molecular analysis and visualization, disentangling spaghetti code into modular framework

Graduate Teaching Assistant August 2019 – May 2020

University of Utah, Department of Chemistry *Salt Lake City, UT*

– Instructed 90+ undergraduate freshmen in General Chemistry Lab I, creating and grading weekly assignments, while maintaining $\geq 95\%$ student satisfaction rating
– Taught Thermodynamics & Kinetics course (51 seniors), providing mentorship on problem-solving and chemical principles, earning Best Teaching Assistant Award (Spring 2020)
– Mentored graduate students on troubleshooting HPC access, SLURM job submissions, and parallel computing workflows

Undergraduate Research Assistant September 2016 – June 2019

Smart Materials Research Institute, Southern Federal University *Rostov-on-Don, Russia*

– Synthesized and characterized 20+ metal-organic framework (MOF) materials for fuel cell applications, utilizing XRD, TEM, SEM, and electrochemical analysis techniques
– Analyzed mass spectrometry and X-ray spectroscopy data from European Synchrotron Radiation Facility (ESRF) experiments on catalytic CO oxidation, contributing to 2 publications
– Developed nitrogen-doped carbon catalysts derived from ZIF precursors, achieving 40% improvement in oxygen reduction reaction (ORR) activity compared to baseline materials
– Delivered 5 peer-reviewed publications on electrocatalyst development and presented research at 4 international conferences, winning Best Poster Award at Faraday Discussion (London, 2018)

Research Collaborator – Synchrotron Experiment Summer 2017

European Synchrotron Radiation Facility (ESRF), BM31 Beamline *Grenoble, France*

– Participated in synchrotron radiation experiments (MA-3676 session) studying catalytic activity of alloyed gold nanoparticles toward CO oxidation using XRPD, EXAFS, and mass spectroscopy
– Prepared samples for high-energy X-ray measurements and monitored real-time data acquisition during 24-hour beamtime sessions
– Processed and analyzed mass spectrometry data using Python, identifying structure-activity relationships in bimetallic nanocatalysts

LEADERSHIP & SERVICE

– Co-Organizer, Machine Learning and Informatics for Chemistry and Materials Workshop, Telluride, CO, USA (2025)

- Led speaker curation and invitations, managed all speaker/venue communications
- Developed the agenda and schedule, facilitated on-site execution
- Initiated a pre-workshop survey to collect participants' opinions, compiled results and guided a group discussion on AI's prospects in the sciences

– Project Mentor at Applied Machine Learning Summer School, Los Alamos National Laboratory, Los Alamos, NM (2025, 2026)
  - Antonio Varagnolo (PhD, Georgia Tech): Active Meta-Learning for Multi-Objective Chemical Search (preprint in prep)
  - Saptati Datta (PhD, Texas A&M): Statistical Insight into Meta-Learning (arXiv preprint)
– AGL Leader, Conference for Undergraduate Women in Physics (CUWiP-2024), Tucson, AZ (2024)
– Discussion Leader, New Understanding of Order Emergence Across Scales, Gordon Research Seminar, Manchester, NH (2023)
– Coordinator, Graduate Research Symposium, University of Utah Department of Chemistry (2023)
– Mentor, Undergraduate Students in Gruenwald Research Group (2021–2022)

EDUCATION

Doctor of Philosophy (PhD) in Physical Chemistry August 2019 – May 2024
University of Utah *Salt Lake City, UT*
– GPA: 3.98/4.0 (Summa Cum Laude) | Advisor: Prof. Michael Gruenwald
– Dissertation: "Computational Insights into the Thermodynamics and Kinetics of Molecular Cocrystallization"

Bachelor of Science (B.Sc.) in Fundamental and Applied Chemistry September 2014 – June 2019
Southern Federal University *Rostov-on-Don, Russia*
– GPA: 4.0/4.0 (Summa Cum Laude) | Honors: Best Undergraduate Thesis (2019)
– Thesis: "Hybrid Zn, Co-ZIF Derived Carbons with Enhanced Catalytic Activity in the Oxygen Reduction Reaction"

PUBLICATIONS

11 total, h-index: 7

- Datta, S., Hengartner, N.W., **Pimonova, Y.**, Klein, N.E., Lubbers, N.E. "Statistical Insight into Meta-Learning via Predictor Subspace Characterization and Quantification of Task Diversity." *arXiv:2509.18349, arXiv*, **15 Jan. 2026**. *arXiv.org*, DOI: 10.48550/arXiv.2509.18349.
- **Pimonova, Y.**, Taylor, M.G., Allen, A.E.A., Yang, P., Lubbers, N.E. "Meta-Learning Linear Models for Molecular Property Prediction." *arXiv:2509.13527, arXiv*, **16 Sept. 2025**. *arXiv.org*, DOI: 10.48550/arXiv.2509.13527.
- Matin, S., Shinkle, E., **Pimonova, Y.**, Craven, G.T., Pachalieva, A., Li, Y.W., Barros, K., Lubbers, N.E. "Ensemble Knowledge Distillation for Machine Learning Interatomic Potentials." *arXiv:2503.14293, arXiv*, **12 June 2025**. *arXiv.org*, DOI: 10.48550/arXiv.2503.14293.
- **Pimonova, Y**; Carpenter, J.E.; Gruenwald, M. "Thermodynamic Stability Is a Poor Indicator of Cocrystallization in Models of Organic Molecules." *Journal of the American Chemical Society*, **2024**, *146*(4), 2805–2815. DOI: 10.1021/jacs.3c13030
- **Pimonova, Y.**; Budnyk, A.; Yohannes, W.; Bugaev, A.; Lastovina, T. "Iron-/Nitrogen-Doped Electrocatalytically Active Carbons for the Oxygen Reduction Reaction with Low Amounts of Cobalt" *ACS Omega*, **2019**, *4*(22), 19548–19555. DOI: 10.1021/acsomega.9b01534
- **Pimonova, Y.**; Lastovina, T.; Budnyk, A.; Kudryavtsev, E.; Yapryntsev, M. "Cobalt-Based ZIF-68 and ZIF-69 as the Precursors of Non-Platinum Electrocatalysts for Oxygen Reduction." *Mendeleev Communications*, **2019**, *29*(5), 544–546. DOI: 10.1016/j.mencom.2019.09.022
- Lastovina, T.; Budnyk, A.; **Pimonova, Y.**; Bugaev, A.; Dmitriev, V. "Thermally-Induced Arrangement of Cobalt and Iron in the ZIF-Derived Fe,Co,Zn-N/C Catalysts for the Oxygen Reduction Reaction." *In-*

ternational Journal of Hydrogen Energy, **2019**, *44 (41)*, 23010-23022. DOI: 10.1016/j.ijhydene.2019.07.022

- Tereshchenko, A.; Polyakov, V.; Guda, A.; Lastovina, T.; **Pimonova, Y.**; Bulgakov, A.; Tarasov, A.; Kustov, L.; Butova, V.; Trigub, A.; Soldatov, A. "Ultra-Small Pd Nanoparticles on Ceria as an Advanced Catalyst for CO Oxidation." *Catalysts*, **2019**, *9 (4)*, 385. DOI: 10.3390/catal9040385
- Nakagame, R.; Tsaturyan, A.; Haraguchi, T.; **Pimonova, Y.**; Lastovina, T.; Akitsu, T.; Shcherbakov, I. "Photochemical Reaction of Amino Acid Schiff Base Derived Cu Complexes with Extended π-System and Their Titanium Oxide Composites." *Inorganica Chimica Acta*, **2019**, *486*, 221–231. DOI: 10.1016/j.ica.2018.10.034
- Lastovina, T.; Budnyk, A.; **Pimonova, Y.**; Bugaev, A.; Fedorenko, A.; Dmitriev, V. "Step-by-Step Synthesis of a Heteroatom-Doped Carbon-Based Electrocatalyst for the Oxygen Reduction Reaction." *Electrochemistry Communications*, **2018**, *88*, 83–87. DOI: 10.1016/j.elecom.2018.02.002
- Lastovina, T.; **Pimonova, J.**; Budnyk, A. "Platinum-Free Catalysts for Low Temperature Fuel Cells." *Journal of Physics: Conference Series*, **2017**, *829*, p. 012007. DOI: 10.1088/1742-6596/829/1/012007

AWARDS & HONORS

Research Awards:

– 2024 Large Team Distinguished Performance Award (*Separation ML Team*) 2025
Los Alamos National Laboratory, NM, USA

– 3MT (Three Minute Thesis) program, Second Prize and Audience Choice Prize 2024
The University of Utah, Salt Lake City, UT, USA

– Poster Prize at the CUP XXII Open Eye's annual scientific meeting 2023
Santa Fe, NM, USA

– Poster Prize at the Berkeley Statistical Mechanics Meeting 2023
Berkeley, CA, USA

– Graduate Research Symposium Outstanding Talk Award 2022
The University of Utah, Salt Lake City, UT, USA

– Graduate Research Conference 20-minute Talk Award 2021
The University of Utah, Salt Lake City, UT, USA

– Best Teaching Assistant of the Semester Award (Thermodynamics & Kinetics Class) 2020
The University of Utah, Salt Lake City, UT, USA

– Best Thesis Project Award 2019
Southern Federal University, Rostov-on-Don, Russia

– Best Poster Presentation at the Designing Nanoparticle Systems for Catalysis, Faraday Discussion 2018
London, UK

– II place at Smart Materials and Mega-Scale Research Facilities School for Young Researchers 2018
Smart Materials Research Institute, Russia

– III place at XXVII Mendeleev's Chemistry Students Contest 2017
Russia

– Student of the Year in Natural Sciences 2017
Southern Federal University, Russia

Scholarships:

– Penny J. Gilmer Grant (CUP XXII Open Eye's annual scientific meeting)
Santa Fe, NM, USA 2023

– Amgen Women in Chemistry Fellowship (Amgen Graduate Student Symposium)
Thousand Oaks, CA, USA 2023

– Advancing Graduate Leadership Scholarship (APS Conference)
Washington D.C., USA 2022

– Air Force Scholarship (American Conference on Theoretical Chemistry)
Palisades Tahoe, NV, USA 2022

SELECTED PRESENTATIONS

– "Adaptive Linear Models via Meta-Learning for Molecular Property Prediction" *Oral*
Machine Learning and Informatics for Chemistry and Materials Workshop, Telluride, CO, USA 2025

– "Adaptive Linear Models via Meta-Learning for Molecular Property Prediction" *Oral*
ACS Fall Meeting, Washington, D.C., USA 2025

– "Introduction to Meta Learning", *Part of Invited Lecture Series* *Oral*
Applied Machine Learning Summer School, Los Alamos National Laboratory, NM, USA 2025

– "Substructural Meta Learning for Interpretable Cheminformatics" *Oral*
Machine Learning and Informatics for Chemistry and Materials Workshop, Telluride, CO, USA 2024

– "Meta Learning Linear Models for Molecular Property Prediction" *Oral*
Applied Machine Learning Summer School, Los Alamos National Laboratory, NM, USA 2023

– "Limits of Cocrystallization Prediction with Supramolecular Synthons and Lattice Energies" *Poster*
Mechanistic Understanding of the Growth and Assembly of Ordered Materials,
Gordon Research Conference, Manchester, NH, USA 2023

– "Can lattice energies and supramolecular synthons predict co-crystallization?" *Oral*
Statistical Thermodynamics & Molecular Simulations Seminar Series, virtual, USA 2023

– "Reimagining Cocrystallization Prediction with Supramolecular Synthons" *Poster*
CUP XXII Open Eye's annual scientific meeting, Santa Fe, NM, USA 2023

– "Computational Insights into Cocrystallization Prediction: From 2D Models to Real Molecules" *Oral*
Amgen Graduate Student Symposium, Thousand Oaks, CA, USA 2023

– "Supramolecular synthons in cocrystallization prediction: From 2D model to real molecule" *Poster*
Berkeley Statistical Mechanics Meeting, Berkeley, CA, USA 2023

– "Molecular Dynamics Simulations of Co-crystallization: Thermodynamics vs. Kinetics" *Oral, Poster*
ACS National Fall Meeting 2022, Chicago, IL, USA 2022

– "Thermodynamic Drive as a Predictor for Molecular Cocrystallization" *Poster*
American Conference on Theoretical Chemistry, Palisades Tahoe, NV, USA 2022

– "Molecular cocrystallization prediction with thermodynamic and kinetic parameters" *Poster*
Berkeley Statistical Mechanics Meeting, virtual, USA 2022

– "ZIF-Derived Co Nanoparticles-Doped Carbons with Enhanced Catalytic Activity in the Oxygen Reduction Reaction" *Poster*
Designing Nanoparticle Systems for Catalysis, Faraday Discussion, London, UK 2019

– "Carbon Materials with Bamboo-Like Nanotubes Active in the Oxygen Reduction Reaction" *Oral*
Smart Materials and Mega-Scale Research Facilities School for Young Researchers,
Smart Materials Research Center, Russia 2018