

## About Yourself:

### 1. Your portrait



### 2. Bio:

- a. Yulia Pimonova is a Postdoctoral Research Associate in the Computing, and Artificial Intelligence (CAI) Division at Los Alamos National Laboratory. In the SeparationML team she develops machine learning approaches to learn from small, experimental datasets to predict high-value separations metrics. She also applies graphlet decomposition analysis to uncover structural and binding motifs across ligand families and metal chemistries, using these insights to propose new ligand designs. Her work sits at the intersection of molecular machine learning, cheminformatics, and molecular simulation, with a focus on uncertainty-aware modeling and data-efficient discovery. Yulia earned her Ph.D. in Physical Chemistry from the University of Utah in May 2024. As a graduate researcher with Dr. Michael Gruenwald, she performed large-scale empirical molecular dynamics simulations of coarse-grained cocrystallization and contributed to advancing cocrystallization theory. Her work has been recognized with multiple honors, including poster prizes at the Berkeley Statistical Mechanics Meeting and OpenEye's annual scientific meeting (both 2023). She is also an active mentor in LANL's Applied Machine Learning Summer Program.
- b.
- c. [https://scholar.google.com/citations?user=e\\_uOeA4AAAAJ&hl=en](https://scholar.google.com/citations?user=e_uOeA4AAAAJ&hl=en)

## About the Project:

1. List for all the publications you have done as part of this project.

- a. **Y Pimonova**, MG Taylor, A Allen, P Yang, N Lubbers “Meta-Learning Linear Models for Molecular Property Prediction.” arXiv:2509.13527, arXiv, 16 Sept. 2025. *arXiv.org*, <https://doi.org/10.48550/arXiv.2509.13527>.
2. The news/highlights (such as C&E News, etc) contributed to this project
  - a. LANL Distinguished Performance Award (team).
3. Description of our unique capabilities and software packages with links:
  - a. minervachem: <https://www.github.com/lanl/minervachem> Interpretable cheminformatics
  - b. minervachem/lamel: <https://github.com/lanl/minervachem/pull/7> Linear Meta-Learning Model for predicting solubilities