

## About Yourself:

1. Your portrait



2. Bio:

- a. Logan Augustine is a Seaborg Postdoctoral Research Fellow in the Physics and Chemistry of Materials (T-1) group at Los Alamos National Laboratory. Within the SeparationML team, Logan has developed Bayesian Optimization techniques to accelerate the discovery of experimental parameters which maximize separations performance in relation to the  $f$ -elements. Along with this, he has conducted computational studies through high-throughput simulation for ligand discovery and the understanding of separation mechanisms. Logan first joined LANL in 2022 as a graduate researcher through a Department of Energy SCGSR fellowship before transitioning to a postdoctoral role in 2023. Before LANL, Logan earned his Ph.D. in chemistry from the University of Iowa, where he was advised by Dr. Sara E. Mason and Dr. Tori Z. Forbes. His doctoral research focused on density functional theory studies of contaminant adsorption at mineral–water interfaces, as well as the vibrational spectroscopy of the neptunyl ion engaged in intermolecular interactions. He received his B.S. in chemistry from Lincoln Memorial University in Tennessee in 2018.

- b.

- c. <https://scholar.google.com/citations?user=2RjSbz8AAAAJ&hl=en>

## About the Project:

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

- a. B. Zhang, T.J. Summers, **L.J. Augustine**, M.G. Taylor, A. Geist, R. Li, E.R. Batista, D. Perez, P. Yang, J. Schrier. "Augmenting Large Language Models for Automated Discovery of f-Element Extractants." *Journal of the American Chemical Society*, 2026, *Accepted*.
  - b. L. da Silva Garcia Leite, B. Zhang, Z. Acar, J. Elowitz, **L.J. Augustine**, A.E. Clark, V. Karamalis, D. Perez, J. Schrier, M.G. Taylor, P. Yang. "Creation of the Separation Archive for Elements (SAFE) Database." *Solvent Extraction and Ion Exchange*, 2025 43(7), 847-852.
  - c. J. Lee, **L.J. Augustine**, G. Henkelman, P. Yang, D. Perez. "Data-Driven Kinetic Reaction Networks for Separation Chemistry." *Journal of Chemical Theory and Computation*, 2025 21(10), 5182-5193.
  - d. T.J. Summers, M.G. Taylor, **L.J. Augustine**, J. Janssen, D. Perez, E.R. Batista, P. Yang. "On the Importance of Configuration Search to the Predictivity of Lanthanide Selectivity." *JACS Au*, 2025, 5(2), 631-641.
  - e. **L.J. Augustine**, Y. Wang, S.L. Adelman, E.R. Batista, S.A. Kozimor, D. Perez, J. Schrier, P. Yang. "Advancing Rare-Earth (4f) and Actinide (5f) Separation through Machine Learning and Automated High-Throughput Experiments." *ACS Sustainable Chemistry & Engineering*, 2024, 12(45), 16692-16699.
  - f. **L.J. Augustine**, J.M. Kasper, T.Z. Forbes, S.E. Mason, E.R. Batista, P. Yang. "Influencing Properties of the Neptunyl(V, VI) Cations with Electron-donating and -withdrawing Groups." *Inorganic Chemistry*, **2023**, 62(15), 6055-6064.
2. *The news/highlights (such as C&E News, etc) contributed to this project.*
    - a. LANL Distinguished Performance Award.
    - b. Seaborg Postdoctoral Research Fellowship - 2024
  3. *Description of our unique capabilities and software packages with links:*
    - a. High-throughput experiment, the LANL Super Separator (videos, etc)
    - b. High-throughput simulation, pyrion/flux interfacing with ADF, Gaussian, VASP
    - c. Architector
    - d. ML- models, PADRE, MLTB, GPR models,
    - e. Cinema visualizer
    - f. Databases for Separation