Nikhil Rampal

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Professional Summary

◇ Computational materials scientist specializing in physics-informed machine learning and atomistic modeling for AI-driven materials discovery. My work focuses on integrating first-principles simulations, molecular dynamics, and machine-learning interatomic potentials with modern AI frameworks to generate high-quality datasets and predictive models for materials design. I develop scalable computational workflows for high-throughput simulations and data generation, enabling large-scale exploration of structure–property relationships across complex materials systems. By combining ab-initio calculations, atomistic simulation, and generative machine learning approaches, I build data-driven models that accelerate materials discovery and support AI-enabled design pipelines. Through close collaboration with machine learning researchers and materials scientists, I translate computational insights into structured datasets and predictive tools that power next-generation generative materials science platforms.

Employment History

2023 – Current ◇ **Postdoctoral Research Fellow**
Quantum Simulations Group,
Laboratory for Energy Applications for the Future (LEAF),
Materials Science Division - Lawrence Livermore National Laboratory.

Education

2018 – 2022 ◇ **Ph.D. Chemical Engineering**, Columbia University in the City of New York.
Exploring Reactivity in Aqueous Solutions and at Mineral-Water Interfaces Through the Lens of Rare Event Theory Atomic Scale Simulations.

Advisors:

- ◇ **Andrew G. Stack** - Distinguished R&D Staff, Group Leader - Geochemistry and Interfacial Sciences Group, Oak Ridge National Laboratory
- ◇ **Sanat K. Kumar** - Michael Bykhovsky and Charo Gonzalez-Bykhovsky Professor of Chemical Engineering, Columbia University

2016 – 2017 ◇ **M.S. Chemical Engineering**, Columbia University in the City of New York.

2011 – 2015 ◇ **B.Tech. Chemical Engineering**, Manipal Institute of Technology.

Awards

◇ **Director's Institutional Award**, Science and Technology - Excellence in Publication, 2025

◇ Physical Life Sciences FY25 Directorate Award for **Outstanding Postdoctoral Fellow**

Technical Expertise

Atomistic Simulation	◇ Classical molecular dynamics, ab initio molecular dynamics (AIMD), density functional theory (DFT), rare-event theory, and enhanced sampling methods.
Machine Learning	◇ Machine-learning interatomic potentials (MLIPs), structure-based property prediction, equivariant graph neural networks, generative models, and physics-informed neural networks for materials discovery.
Experimental Integration	◇ Integration of simulations with neutron scattering, synchrotron X-ray techniques, and operando characterization to validate atomic-scale mechanisms.
Software	◇ LAMMPS, VASP, PLUMED, CP2K, ASE, PyTorch, NequIP/MACE-style equivariant models.

Mentorship

Jun 2025 – Current	◇ Srikant Sagireddy, Ph.D, Stanford University. **Leveraging foundation model for battery electrolyte design.**
Jun 2024 – Current	◇ Jaeyoung Cho, Ph.D, University of Texas, Austin. **Atomistic elucidation of phase evolution mechanism in crystalline BN.**
Jun 2024 – Sept 2024	◇ Nihang Fu, Ph.D., University of South Carolina. **Machine learning for electrolyte design.**
Oct 2023 – Feb 2024	◇ Yu Zhang, Ph.D., University of Pittsburgh. **Lithium electrolyte decomposition at the Li-metal interface using first-principles calculations.** *Currently a Postdoctoral Scholar at Caltech with Prof. Anima Anandkumar*

Research Publications

Journal Articles

1. **Rampal**, **N.**, Weitzner, S. E., Omenya, F., Wood, M., Reed, D. M., Li, X., Lee, J. R. & Wan, L. F. Physics-informed machine learning exploration of Na storage mechanisms in disordered carbon. *Energy Storage Materials,* 104967 (2026).
2. Yuan, K., Weber, J., **Rampal**, **N.**, Fang, Z., You, J., Boebinger, M. G., Zhang, R., Cha, W., Anovitz, L. M., Lee, S. S., *et al.* Mechanistic Insights into Defect-Mediated Crystallization Revealed by Lattice Strain Evolution. *Journal of the American Chemical Society* (2026).
3. Bunting, R. J., Shepherd, S., **Rampal**, **N.**, Akhade, S., Wilkins, D. M. & Pham, T. A. Nuclear quantum effects of metal surface-mediated C–H activation. *Physical Chemistry Chemical Physics* **27,** 16051–16056 (2025).
4. Weitzner, S. E., Wang, B., **Rampal**, **N.**, Jeong, W., Yuan, S., Zhang, S., Bucci, G., Adelstein, N., Yan, S., Marschilok, A. C., *et al.* Cross-Scale Modeling and Experimental Integration for Advancing Cathode Electrolyte Interphase Studies in High Energy Density Lithium-Ion Batteries. *Energy Storage Materials,* 104368 (2025).

5. Kitsu Iglesias, L., Marks, S. D., **Rampal**, **N.**, Antonio, E. N., de Ferreira de Menezes, R., Zhang, L., Olds, D., Weitzner, S. E., Sprenger, K. G., Wan, L. F., *et al.* Microstructure-Dependent Sodium Storage Mechanisms in Hard Carbon Anodes. *Small,* 2505561 (2025).

6. You, J., Yuan, K., **Rampal**, **N.**, Stack, A. G. & Starchenko, V. How are Heterogeneous Nucleation Rate Observations Influenced by Instrument Resolution? *ACS Applied Materials & Interfaces* **17,** 17492–17500 (2025).

7. Yuan, K., **Rampal**, **N.**, Adapa, S., Evans, B. R., Bracco, J. N., Boebinger, M. G., Stack, A. G. & Weber, J. Iron Impurity Impairs the CO_2 Capture Performance of MgO: Insights from Microscopy and Machine Learning Molecular Dynamics. *ACS Applied Materials & Interfaces* **16,** 64233–64243 (2024).

8. **Rampal**, **N.**, Weitzner, S. E., Cho, S., Orme, C. A., Worsley, M. A. & Wan, L. F. Structural and transport properties of battery electrolytes at sub-zero temperatures. *Energy & Environmental Science* (2024).

9. Butreddy†, P., Heo†, J., **Rampal, N.**†, Liu, T., Liu, L., Smith, W., Zhang, X., Prange, M. P., Legg, B. A., Schenter, G. K., De Yoreo, J. J., Chun, J., Stack, A. G. & Nakouzi, E. Ion Correlations Decrease Particle Aggregation Rate by Increasing Hydration Forces at Interfaces. *ACS nano* (2024).

10. Yuan, K., **Rampal**, **N.**, Du, X., Shu, F., Wang, Y., Wang, H., Stack, A. G., Ishai, P. B., Anovitz, L. M. & Xu, P. Impact of magnetic and electric fields on the free energy to form a calcium carbonate ion-pair. *Physical Chemistry Chemical Physics* (2024).

11. Yuan, K., **Rampal**, **N.**, Irle, S., Criscenti, L. J., Lee, S. S., Adapa, S. & Stack, A. G. Variations in proton transfer pathways and energetics on pristine and defect-rich quartz surfaces in water: Insights into the bimodal acidities of quartz. *Journal of Colloid and Interface Science* **666,** 232–243 (2024).

12. Liu, T., **Rampal**, **N.**, Nakouzi, E., Legg, B. A., Chun, J., Liu, L., Schenter, G. K., De Yoreo, J. J., Anovitz, L. M. & Stack, A. G. Molecular Mechanisms of Sorbed Ion Effects during Boehmite Particle Aggregation. *Langmuir* **40,** 8791–8805 (2024).

13. **Rampal**, **N.**, Wang, H.-W., Brady, A. B., Borreguero, J. M., Biriukov, D., Mamontov, E. & Stack, A. G. Testing the hypothesis that solvent exchange limits the rates of calcite growth and dissolution. *RSC advances* **14,** 15743–15754 (2024).

14. Yuan, K., Starchenko, V., **Rampal**, **N.**, Yang, F., Xiao, X. & Stack, A. G. Assessing an aqueous flow cell designed for in situ crystal growth under X-ray nanotomography and effects of radiolysis products. *Journal of Synchrotron Radiation* **30,** 634–642 (2023).

15. Dhakal, D., Driscoll, D. M., Govind, N., Stack, A. G., **Rampal**, **N.**, Schenter, G., Mundy, C. J., Fister, T. T., Fulton, J. L., Balasubramanian, M., *et al.* The evolution of solvation symmetry and composition in Zn halide aqueous solutions from dilute to extreme concentrations. *Physical Chemistry Chemical Physics* **25,** 22650–22661 (2023).

16. Brady, A. B., Weber, J., Yuan, K., Allard, L. F., Avina, O., Ogaz, R., Chang, Y.-J., **Rampal**, **N.**, Starchenko, V., Rother, G., *et al.* In situ observations of barium sulfate nucleation in nanopores. *Crystal Growth & Design* **22,** 6941–6951 (2022).

17. Yang, P., **Rampal**, **N.**, Weber, J., Bracco, J. N., Fenter, P., Stack, A. G. & Lee, S. S. Synergistic Enhancement of Lead and Selenate Uptake at the Barite (001)–Water Interface. *Environmental Science & Technology* **56,** 16801–16810 (2022).

18. Biriukov, D., Wang, H.-W., **Rampal**, **N.**, Tempra, C., Kula, P., Neuefeind, J. C., Stack, A. G. & Předota, M. The "good," the "bad," and the "hidden" in neutron scattering and molecular dynamics of ionic aqueous solutions. *The Journal of Chemical Physics* **156** (2022).

19. Anovitz, L. M., Huestis, P., **Rampal**, **N.**, Stack, A. G., LaVerne, J., Zhang, X., Schenter, G., Chun, J., Legg, B., Liu, L., *et al.* Frustrated Coulombic and cation size effects on nanoscale boehmite aggregation: A tumbler small-and ultra-small-angle neutron scattering study. *The Journal of Physical Chemistry C* **126,** 4391–4414 (2022).

20. Wang, H.-W., Yuan, K., **Rampal**, **N.** & Stack, A. G. Solution and interface structure and dynamics in geochemistry: Gateway to link elementary processes to mineral nucleation and growth. *Crystal Growth & Design* **22,** 853–870 (2021).

21. **Rampal**, **N.**, Wang, H.-W., Biriukov, D., Brady, A. B., Neuefeind, J. C., Předota, M. & Stack, A. G. Local molecular environment drives speciation and reactivity of ion complexes in concentrated salt solution. *Journal of Molecular Liquids* **340,** 116898 (2021).

22. Yuan, K., **Rampal**, **N.**, Fenter, P., Kubicki, J. D., Stack, A. G. & Irle, S. Density functional tight-binding simulations reveal the presence of surface defects on the quartz (101)–water interface. *The Journal of Physical Chemistry C* **125,** 16246–16255 (2021).

23. Yuan, K., Starchenko, V., **Rampal**, **N.**, Yang, F., Yang, X., Xiao, X., Lee, W.-K. & Stack, A. G. Opposing effects of impurity ion Sr2+ on the heterogeneous nucleation and growth of barite ($BaSO_4$). *Crystal growth & design* **21,** 5828–5839 (2021).

Preprints

1. Sagireddy†, S., **Rampal, N.**†, Weitzner, S. E. & Wan, L. F. *Integrated Machine Learning-Molecular Dynamics Framework for Electrolyte Property Prediction* **Accepted**.

2. Yuan†, S., **Rampal, N.**, Adelstein, N. & Wan, L. F. *Elucidating Li transport mechanism in disordered LiF from machine-learning molecular dynamic simulations* **Under Review**.

3. **Rampal**, **N.**, Weitzner, S. E., Sun, W., Hollas, A., Murugesan, V., Reed, D. M., van Buuren, T., Lee, J. R. I. & Wan, L. F. *Nanoscale Structural and Transport Fluctuations in the Electric Double Layer: Critical Drivers of Vanadium Redox Flow Battery Performance* **Under Internal Review**.

4. **Rampal**, **N.**, Weitzner, S. E., Cho, S., Orme, C. A., Worsley, M. A. & Wan, L. F. *Resolving Competing Effects in Battery Systems via Atomistic Simulations* **Under Internal Review**.

5. Singh, S., Paul, R., **Rampal**, **N.**, Bunting, R. J., Hamel, S., Pulver, N., McGuire, C. P., Clarke, S. M., Coleman, A., Vennari, C., Hutchinson, T. M., Periera, K. A., Naglar, B., Khaghani, D., Lee, H. J., McGonegle, D., Volz, T., OCampo, I. K., McNaney, J., Lockard, T., Eggert, J. H., Krygier, A. & Smith, R. F. *High pressure phase stability and melt in shock-compressed titanium* **Submitted**.

6. **Rampal**, **N.**, Wang, H.-W., Ke, Y. & Stack, A. G. *Saturation Dependent Nucleation Pathways and Phase Transitions.* **In preparation**.

Conference Proceedings

1. **Rampal**, **N.**, Wang, H.-W., Yuan, K. & Stack, A. *Beyond Classical Nucleation Theory: Molecular Insights into Non-Classical Pathways of Sparingly Soluble Salts* in *American Conference of Crystal Growth and Epitaxy.* **Session Chair and Speaker** (2025).

2. **Rampal**, **N.** *Ionic and Microstructural Mechanisms in Next-Generation Energy Storage Materials* in *San Francisco State University* **Invited** (2025).

3. **Rampal**, **N.**, Weitzner, S. E., Cho, S., Orme, C. A., Worsley, M. A. & Wan, L. F. *Design Principles for High-Performance Electrolytes—Overcoming Low-Temperature Challenges in Lithium-Ion Batteries* in *Materials Research Society* (2025).

4. **Rampal**, **N.**, Adelstein, N., Sun, W., Weitzner, S. E., Orme, C. A., Worsley, M. A. & Wan, L. F. *Decoding the mechanistic processes that dictate battery performance using enhanced sampling simulations* in *Abstracts of Papers of the American Chemical Society* (2024).

5. **Rampal**, **N.**, Kroutil, O., Wang, H.-W., Mamontov, E., Biriukov, D., Predota, M. & Stack, A. *Structure and dynamics of water on Calcite (104) surface studied by quasielastic neutron scattering and molecular dynamics simulations* in *Abstracts of Papers of the American Chemical Society* (2021).

6 **Rampal**, **N.**, Wang, H.-W., Biriukov, D., Brady, A., Neuefeind, J., Predota, M. & Stack, A. *Amalgamation of computational and experimental studies to probe the effect of local molecular environments in aqueous salt solutions* in *Pacifichem* **Invited** (2021).

7 **Rampal**, **N.**, Wang, H.-W., Stack, A., Biriukov, D. & Neuefeind, J. *Chloride ion solvation, dynamics and ion-pairing interactions in concentrated aqueous solutions: Combined computational simulation and neutron diffraction with isotopic substitution* in *Abstracts of Papers of the American Chemical Society* **257** (2019).