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Muhammad Risyad Hasyim

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Education

The University of California, Berkeley *8/2017 - 8/2023*
Ph.D. in Chemical Engineering

- **Thesis:** Understanding Glassy Dynamics in Supercooled Liquids
- **Awards:** Berkeley Fellowship for Graduate Study; Oral Presentation Prize at Fall 2022 MRS Meeting

The Pennsylvania State University *8/2013 - 5/2017*
B.Sc.(Hons) in Chemical Engineering, Minor in Mathematics

- **Thesis:** Mathematical Modeling of Electrochemical Capacitors
- **Award:** The Peter T. Luckie Award for best research poster

B.Sc.(Hons) in Engineering Science

- **Thesis:** Experimental Studies and Modeling of Lithium Borate-Silica Composite Solid Electrolyte
- **Award:** The Francis H. Fenlon Award for best thesis

Professional Experience

Postdoctoral Fellow *New York, NY*
New York University, Department of Chemistry *8/2023 - Present*

- Simons Postdoctoral Fellowship recipient ($10,000/yr discretionary funds) conducting independent research in the areas of computational chemistry, such as machine learning (ML) for molecular simulations.
- Contributed to Open Molecules 2025 (OMol25), a 100M+ computational chemistry dataset for training foundational ML models in collaboration with Meta FAIR Chemistry, academic, industrial, and national laboratory partners.
- Designed and executed automated molecular dynamics pipelines for randomized electrolyte mixtures using LAMMPS, Desmond, and OpenMM, including ring polymer molecular dynamics simulations.
- Trained E(3)-equivariant neural networks (e3nn architecture) on small molecule datasets to predict electron densities and molecular energies for computational spectroscopy applications.
- Developed JIT-compiled physics simulation code for light-matter systems using mixed quantum-classical methods, achieving production-ready performance for cavity chemistry predictions.
- Built GPU-accelerated molecular dynamics code (cav-hoomd) coupling electromagnetic fields with particle simulations for quantum materials research.

Scientific Consultant *Remote*
Self-Employed *2/2025 – Present*

- Generated $23,000+ in one year providing ML and scientific computing consulting across AI, energy, and pharmaceutical sectors.
- Built end-to-end computational drug screening pipeline, combining ML models (AlphaFold for structure prediction, DiffDock for binding, ADMET-AI for properties) with molecular simulation tools (RDKit, OpenMM).
- Developed physics-informed ML models for battery optimization and electrolyzer design using differentiable simulation frameworks (PyBAMM/PyBOP) and finite element methods (COMSOL).
- Prototyped agentic AI system for polymeric materials discovery using LangChain with MCP tool integration for autonomous literature search and property prediction.

Graduate Student Research Assistant *Berkeley, CA*
UC - Berkeley, Department of Chemical and Biomolecular Engineering *8/2017 – 8/2023*

- Developed GPU-accelerated scientific computing infrastructure (C++/CUDA) for large-scale Monte Carlo and molecular dynamics simulations, achieving 10-100x speedup over CPU baselines.
- Engineered distributed parallel sampling algorithm (MPI-based) achieving 10x acceleration for rare event sampling in glassy systems across multi-node HPC clusters.
- Trained deep neural networks (PyTorch) to learn transition probabilities (committor functions) from simulation data, enabling ML-accelerated rare event prediction with 100-1000x speedup vs. traditional methods.

Publications in Preparation

** denotes machine learning-focused publications*

[1] *Bogojeski, M., **Hasyim, M.R.**, Vogt-Maranto, L., Müller, K.-R., Burke, K., and Tuckerman, M. E. "Enhancing molecular dynamics with equivariant machine-learned densities". In Prep. Jan. 2026.

[2] Song, S., Fernandes, J. B., **Hasyim, M.R.**, and Mandadapu, K. K. "Dynamical scaling of coarsening domains in relaxing supercooled liquids". In Prep. Jan. 2026.

[3] **Hasyim, M.R.**, Damiani, A., and Hoffmann, N. M. "Non-thermal aging and cooling of supercooled liquids in microcavities". In Prep. Dec. 2025.

[4] **Hasyim, M.R.**, Garrahan, J. P., and Mandadapu, K. K. "Glassy dynamics of supercooled liquids". **Invited** review for the *Annual Review of Physical Chemistry*; In Prep. June 2026.

Published Publications

[5] *Levine, D., Shuaibi, M., Spotte-Smith, E., Taylor, M., **Hasyim, M.R.**, Michel, K., Batatia, I., Csányi, G., Dzamba, M., Eastman, P., Frey, N., Fu, X., Gharakhanyan, V., Krishnapriyan, A., Rackers, J., Raja, S., Rizvi, A., Rosen, A., Ulissi, Z., Vargas, S., Zitnick, C., Blau, S., and Wood, B. "The Open Molecules 2025 (OMol25) dataset, evaluations, and models". In: (May 2025). Submitted to *Science*. arXiv: 2505.08762 [physics.chem-ph]. URL: https://arxiv.org/abs/2505.08762.

[6] **Hasyim, M.R.**, Mandal, A., and Reichman, D. R. "Towards accurate mixed quantum-classical simulations of vibrational polaritonic chemistry". In: (Feb. 2025). **Invited** to *The Journal of Chemical Physics*. arXiv: 2502.04570 [quant-ph].

[7] **Hasyim, M.R.** and Mandadapu, K. K. "Theory of crystallization versus vitrification". In: (Dec. 2025). Submitted to *Physical Review X*. arXiv: 2007.14968 [cond-mat.stat-mech].

[8] **Hasyim, M.R.** and Mandadapu, K. K. "Emergent facilitation and glassy dynamics in supercooled liquids". In: *Proceedings of the National Academy of Sciences* 121.23 (Apr. 2024), e2322592121. DOI: 10.1073/pnas.2322592121.

[9] Fraggedakis, D., **Hasyim, M.R.**, and Mandadapu, K. K. "Inherent-state melting and the onset of glassy dynamics in two-dimensional supercooled liquids". In: *Proceedings of the National Academy of Sciences* 120.14 (Feb. 2023), e2209144120. DOI: 10.1073/pnas.2209144120.

[10] ***Hasyim, M.R.**, Batton, C. H., and Mandadapu, K. K. "Supervised learning and the finite-temperature string method for computing committor functions and reaction rates". In: *The Journal of Chemical Physics* 157.18 (Nov. 2022), p. 184111. DOI: 10.1063/5.0102423.

[11] **Hasyim, M.R.** and Mandadapu, K. K. "A theory of localized excitations in supercooled liquids". In: *The Journal of Chemical Physics* 155.4 (July 2021). ***Selected as Editor's Pick and JCP Editor's Choice 2021***, p. 044504. DOI: 10.1063/5.0056303.

[12] **Hasyim, M.R.** and Rajagopalan, R. "Prediction of discharge performances of pseudocapacitors using their impedance characteristics". In: *Journal of the Electrochemical Society* 167.1 (Jan. 2020), p. 013536. DOI: 10.1149/1945-7111/ab6722.

[13] **Hasyim, M.R.** and Lanagan, M. T. "A new percolation model for composite solid electrolytes and dispersed ionic conductors". In: *Modelling and Simulation in Materials Science and Engineering* 26.2 (Jan. 2018), p. 025011. DOI: 10.1088/1361-651x/aaa26f.

[14] **Hasyim, M.R.**, Ma, D., Rajagopalan, R., and Randall, C. "Prediction of charge-discharge and impedance characteristics of electric double-layer capacitors using porous electrode theory". In: *Journal of the Electrochemical Society* 164.13 (Sept. 2017), A2899–A2913. DOI: 10.1149/2.0051713jes.

[15] **Hasyim, M.R.**, Berbano, S. S., Cleary, R. M., Lanagan, M. T., and Agrawal, D. K. "Impedance spectroscopy modeling of lithium borate with silica: A dispersed ionic conductor system". In: *Ceramics International* 43.9 (June 2017), pp. 6796–6806. DOI: 10.1016/j.ceramint.2017.02.097.

Selected Talks

[16] **Hasyim, M.R.** "Excitations, emergent facilitation, and glassy dynamics in supercooled liquids". In: 10th International Discussion Meeting on Relaxations in Complex Systems (10^{th} IDMRCS). (Oral, **Invited**) Barcelona, Spain, July 2025.

[17] **Hasyim, M.R.** "Polariton-induced modifications to relaxation and transport in supercooled liquids". In: CCQ-NYU Light-Matter Seminar. (Oral, **Invited**) New York, NY, Mar. 2025.

[18] **Hasyim, M.R.** "Understanding cavity-mediated dynamics in vibrational polaritonic chemistry". In: Virtual International Seminar on Theoretical Advancements (VISTA). (Oral, **Invited**) Virtual: Link, Mar. 2025.

[19] **Hasyim, M.R.**, Hoffmann, N., Mandal, A., and Reichman, D. R. "Excursions in vibrational polaritonic chemistry: from relaxation in liquids to chemical kinetics". In: The 11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP). (Oral) Qingdao, China, Oct. 2024.

[20] **Hasyim, M.R.** "A theory of localized excitations and onset temperature in supercooled liquids". In: The Pitzer Seminar for Theoretical Chemistry. (Oral, **Invited**) Berkeley, CA, Sept. 2022.

[21] **Hasyim, M.R.** "A theory of localized excitations and onset temperature in supercooled liquids". In: Special Seminar at the University of Cambridge, UK. (Oral, **Invited**) Virtual, Sept. 2022.

[22] **Hasyim, M.R.** "A theory of localized excitations and onset temperature in supercooled liquids". In: Special Seminar at Stanford University. (Oral, **Invited**) Stanford, CA, Aug. 2022.

[23] **Hasyim, M.R.** "A theory of localized excitations and onset temperature in supercooled liquids". In: Theory Club at Université Paris Diderot, France. (Oral, **Invited**) Virtual, July 2022.

Open Source Projects

cav-hoomd (☆ 1) – A plugin to HOOMD-blue for performing classical molecular dynamics (MD) simulations coupled to cavity electromagnetic fields with GPU acceleration.

tps-torch (☆ 3 ⑂ 1) – A PyTorch-based package for string methods and ML-inspired path sampling methods.

pyglasstools (☆ 2) – Data analysis package for calculating properties of amorphous materials. Interfaced with PETSc/SLEPc (multi-CPU Fortran/C algebra packages).

pyfdam (☆ 4) – a lightweight Python library to fit linear electrochemical models to experimental impedance spectroscopy data and predict energy and power density of real devices.

boltz-demo – Interactive HuggingFace Space demonstrating Boltz-2 for biomolecular structure prediction.

om-data (OMol25) (☆ 15 ⑂ 5) – Repository for generating inputs and scripts in the Open Molecules 2025 dataset. Contributed in creating end-to-end pipeline for molecular dynamics of randomized electrolyte mixtures.

equiv_dens_ml – E(3) equivariant neural networks for electron density-based machine learning force fields. Wrote evaluation scripts, specifically for infrared spectroscopy calculations.

parallel-swap-mc (☆ 3) – A plug-in for HOOMD-Blue that allows parallel Monte Carlo simulation of soft & hard continuous-polydisperse particles on CPUs.

Peer Review

Digital Discovery (Impact Factor: 6.2)	8/2023 - Present
Physical Review E (Impact Factor: 2.2)	8/2024 - Present
Reports on Progress in Physics (Impact Factor: 19.0)	5/2025 - Present
New Journal of Physics (Impact Factor: 2.8)	8/2025 - Present

Skills & Technologies

Programming: C/C++, Python, Mathematica, MATLAB, CMake/Make, Bash, Vi/Vim, Git

HPC: OpenMP, OpenMPI, CUDA, SGE/PSB, SLURM,

Machine Learning & Optimization: PyTorch, PyBOP, scikit-learn, scikit-optimize, PuLP

AI Engineering: Cursor, `mcp`, LangChain

Molecular Simulations: HOOMD-Blue, LAMMPS, OpenMM, Desmond, ASE

Electronic Structure: PySCF, ORCA, CP2K

Molecular Visualization: Avogadro, Ovito

Finite Element Analysis: COMSOL, PyBAMM, PETSc/SLEPc, FEniCSx

Markup Languages: LaTeX, Markdown, RMarkdown, Hugo

Graphical Design: Tikz-LaTeX, gnuplot, Matplotlib, Inkscape, Adobe Illustrator

Languages: English (full professional proficiency), Bahasa Indonesia (native or bilingual proficiency)