Muhammad Risyad Hasyim

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muhammadhasyim

Summary

Versatile computational scientist with 10+ years of experience in scientific computing, finite element analysis, machine learning, quantum chemistry, and molecular simulations. Proficient in C++/Python scientific stack and domain-specific tools to deliver computational solutions and consulting services in physics-based machine learning, energy storage modeling, and computational drug discovery.

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*

- Funded by the Simons Postdoctoral Fellowship for Computational Physical Chemistry ($82,000/year contract with $10,000 funding) to perform independent research on the field of theoretical chemistry.
- Investigated the feasibility of catalyzing reactions using quantum vacuum-field and thermal fluctuations of electromagnetic fields, via mixed quantum-classical methods.
- Collaborated with the FAIR Chemistry team at Meta and other academic institutions to generate a new dataset to train foundational AI models for chemistry (Open Molecules 2025, project on-going).

Scientific Consultant *Remote*
Self-Employed *2/2024 – Present*

- Generated $7,300+ in 2.5 months providing scientific consulting in artificial intelligence (AI), energy, and pharmaceutical sectors.
- Modeled energy storage devices such as fuel cells, electrolyzers, and lithium-ion batteries using Python software stack (PyBAMM/PyBOP) and finite element analysis (COMSOL).
- Built computational drug discovery pipeline integrating protein structure loading, molecular docking, and ADMET analysis using AlphaFold, RDKit, RCSB API, OpenMM, and DiffDock.
- Delivered physics-based machine learning solutions for applications ranging from sensor technologies to fraud detection.

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

- Developed GPU-accelerated scientific (C++/CUDA) code to perform Monte Carlo (MC) and molecular dynamics (MD) simulations.
- Used MC and MD simulations to study how supercooled liquids form solid glasses.
- Created novel machine learning algorithm using PyTorch to sample rare events in molecular simulations.

Publications

[1] **Hasyim, M. R.**, Arkajit Mandal, and David R. Reichman. "Towards accurate mixed quantum classical simulations of vibrational polaritonic chemistry". In: (Feb. 2025). arXiv: 2502.04570 [quant-ph].

[2] **Hasyim, M. R.** and Kranthi K Mandadapu. "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.

[3] D. Fraggedakis, **Hasyim, M. R.**, and Kranthi K. Mandadapu. "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.

[4] **Hasyim, M. R.**, Clay H Batton, and Kranthi K Mandadapu. "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.

[5] **Hasyim, M. R.** and Kranthi K Mandadapu. "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.

[6] **Hasyim, M. R.** and Kranthi K. Mandadapu. "Theory of crystallization versus vitrification". In: (July 2020). arXiv: 2007.14968 [cond-mat.stat-mech].

[7] **Hasyim, M. R.** and Ramakrishnan Rajagopalan. "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.

[8] **Hasyim, M. R.** and Michael T Lanagan. "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.

[9] **Hasyim, M. R.**, Seth S Berbano, Regis M Cleary, Michael T Lanagan, and Dinesh K Agrawal. "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.

[10] **Hasyim, M. R.**, Danhao Ma, Ramakrishnan Rajagopalan, and Clive Randall. "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.

Peer Review

Digital Discovery (Impact Factor: 6.2) 8/2023 - Present
Physical Review E (Impact Factor: 2.2) 8/2024 - Present

Skills & Technologies

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

Markup Languages: LaTeX, Markdown, RMarkdown, Hugo

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

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

Machine Learning: PyTorch, scikit-learn

Finite Element Analysis: COMSOL, PETSc/SLEPc, FEniCSx

Visualization & Design: Tikz-LaTeX, gnuplot, Matplotlib, Ovito, Inkscape, 5Adobe Illustrator

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