YUE (SAMUEL) YU

New Haven, CT | (+1) 475-301-9267 | samuel.yu@yale.edu | linkedin.com/in/samuel-yue-yu-b0652593/

Ph.D. candidate in computational molecular science, quantum machine learning, and large-scale simulation, with training in biophysics and nonequilibrium molecular dynamics. Interested in molecular dynamics, enhanced sampling, statistical-mechanical free energies, and solvent-mediated protein allostery.

EDUCATION

Yale University | New Haven, CT July 2022–present (expected May 2028)

Ph.D. candidate, Engineering & Applied Science (Mechanical Engineering & Materials Science) | Advisor: Prof. Victor S. Batista

M.Phil. (2025) and M.S. (2023; GPA 4.00/4.00), Engineering & Applied Science

Certificate, Integrated Graduate Program in Physical & Engineering Biology (2026)

Duke Kunshan University / Duke University | Kunshan, China / Durham, NC August 2018–May 2022

B.S., Molecular Bioscience (Duke Kunshan University; GPA 3.972/4.000); B.S., Molecular Bioscience, Biophysics track (Duke University; GPA 4.00/4.00)

Undergraduate thesis: “Size-Sieving Separation of Hard-Sphere Mixtures through Cylindrical Pores” | Advisor: Prof. Kai Zhang

RESEARCH EXPERIENCE

Graduate Researcher — Batista Research Group, Yale University 2022–present

- Developed **QOBRA**, a Quantum Operator-Based Autoencoder for de novo molecular design, linking quantum machine-learning methodology with molecular representations and rigorous computational benchmarking (published in *J. Chem. Theory Comput.*, 2026); extended the approach to a fully quantum framework for protein sequence design.
- Predicted Mn-protein structures with AlphaFold3 and PyMOL to set up QM/MM free-energy cycle calculations for Mn(II/III)P–BIPH, in collaboration with Arizona State University.
- Lead the **QuantumCT** seed project, integrating QOBRA into hybrid quantum–classical AI for cardiovascular drug design and cardiotoxicity prediction; coordinate team meetings, records, and progress reports.
- Developed **Qydra**, a multi-headed hybrid quantum–classical virtual cell for the Arc Institute Virtual Cell Challenge 2026 that predicts single-cell transcriptomic responses to CRISPRi knockdowns in unseen cell lines; it merges a QOBRA-style quantum circuit head with measured transfer from public CRISPRi screens, gated per cell context by a quantum autoencoder trained on control cells.
- Implemented quantum machine-learning workflows on Quantinuum H1-1 hardware; evaluated device noise, finite-sampling effects, and calibration-based confusion-matrix readout-error mitigation for generated protein structures.
- Applied **probabilistic error cancellation (PEC)** to a two-qubit Hamiltonian VQE circuit with collaborators at the Universities of Pittsburgh, Michigan, and Helsinki; contributed the PEC material to the quantum error mitigation chapter of the **QFlux** open-source quantum dynamics tutorial.
- Conducted large-scale computational experiments and systematic benchmarking using National Energy Research Scientific Computing Center (NERSC) Perlmutter resources.

Early Talent Intern, Molecular AI — Novo Nordisk R&D US, Inc. | Lexington, MA June–August 2026

- Extended the QOBRA quantum variational autoencoder to generate molecules with specified drug-relevant chemical properties, applying machine-learning- and quantum-informed approaches in an interdisciplinary pharmaceutical research environment; results submitted to ICLR 2027.

Summer Research Scholar — Myung-Joong Hwang Research Group | Duke Kunshan University May–Aug. 2021

- Investigated quantum entanglement in two coupled identical Rabi models near the normal-to-superradiant transition; identified a superradiant regime with zero entanglement (ground-state factorization) and compared quantum (anti-)Jaynes–Cummings and Dicke models.
- Identified possible emergence of continuous symmetry in large Dicke lattice systems with long-range interactions (arXiv:2510.08391).

Research Assistant — Kai Zhang Research Group | Duke Kunshan University Feb. 2019–Apr. 2021

- Studied size-dependent transport and separation of hard-sphere mixtures through cylindrical pores using nonequilibrium event-driven molecular dynamics and analytical collision dynamics; showed that permeability follows a hindered-diffusion mechanism arising from size exclusion (published in *Soft Matter*, 2021).
- Developed C++ simulation workflows in Linux and analyzed results using Jupyter notebooks; investigated power-law permeability and selectivity relationships; shared simulation code on GitHub.

PUBLICATIONS & PREPRINTS

1. **Yu, Y.**, Calcagno, F., Li, H., and Batista, V. S. “QOBRA: A Quantum Operator-Based Autoencoder for De Novo Molecular Design.” *Journal of Chemical Theory and Computation* 22 (4), 2059–2073 (2026). doi:10.1021/acs.jctc.5c01704
2. **Yu, Y.**, and Hwang, M.-J. “Emergent Continuous Symmetry and Ground-State Factorization Induced by Long-Range Interactions.” arXiv:2510.08391 (2025).
3. **Yu, Y.**, Wang, R., and Teo, R. D. “Machine Learning Approaches for Metalloproteins.” *Molecules* 27 (4), 1277 (2022). doi:10.3390/molecules27041277
4. **Yu, Y.**, and Zhang, K. “Size-Sieving Separation of Hard-Sphere Gases at Low Concentrations through Cylindrically Porous Membranes.” *Soft Matter* 17 (44), 10025–10031 (2021). doi:10.1039/d1sm01158h

PRESENTATIONS

Invited talks — “QOBRA: A Quantum Operator-Based Autoencoder for De Novo Molecular Design.” 10th Yale Annual Biophysics and Structural Biology Symposium (2025); Envisioning AI at Yale: An Interdisciplinary Symposium (2025).

Oral presentation — “Molecular Simulation of Gas Transport Through Cylindrical Pores.” American Physical Society March Meeting, Session J21 (virtual), March 2021.

Posters (QOBRA) — Monterey Data Conference, NERSC (2025); Find Your Inner Modeler Conference, UC Irvine (2025); NYC AI4Chemistry Summit, NYU (2025); 9th Yale Annual Biophysics and Structural Biology Symposium (2024).

TEACHING, LEADERSHIP & SERVICE

Graduate Teaching Assistant — Thermodynamics for Mechanical Engineers, Yale Spring 2024

- Assisted Prof. Alessandro Gomez with tutoring, solutions, grading, and exam proctoring; led a weekly 1.25-hour practice-problem session.

Research Computing & Industry Liaison — Batista Research Group2024–present

- Prepare NERSC Perlmutter allocation applications and manage group computing resources; communicate with industrial partners in quantum computing and pharmaceuticals.

Advanced Graduate Leadership Program, Yale — Venture track for industrial leadership2025–present

Undergraduate Peer Tutor — Intro. to Statistics & Data Science, Duke Kunshan Spring 2019

COMPUTATIONAL EXPERTISE

Molecular simulation & structure: molecular and event-driven dynamics; OpenMM; QM/MM free-energy cycles; AlphaFold3; PyMOL; VMD; RDKit; Biopython

Machine learning & quantum: generative molecular modeling; quantum–classical algorithms; variational quantum circuits; quantum-hardware benchmarking and error mitigation (readout mitigation, PEC); PyTorch; scikit-learn; Qiskit; TorchQuantum; Quantinuum H1-1

Computing: Python; C/C++; R; Java; CUDA; Linux; Jupyter notebooks; high-performance computing (NERSC Perlmutter); statistical analysis and reproducibility

RESEARCH INTERESTS

Solvent-aware protein networks, hydration-site statistics, enhanced sampling, free-energy convergence, joint solvation interactions, and computational–experimental studies of phosphatase allostery.