Romit Chakraborty, Ph.D.

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Professional Profile

Quantum Chemist and AI Researcher with extensive expertise in fault-tolerant quantum computing (FTQC), physics-grounded generative modelling, and domain-specific algorithm adaptation. Proven track record of bridging advanced theoretical methods and real-world computational bottlenecks by engineering performant simulation pipelines, developing analytical resource models, and conducting rigorous classical-versus-quantum benchmarking. Experienced technical communicator skilled at translating complex algorithmic metrics into reproducible evidence for cross-functional partners and domain experts.

Key Skills & Tools

2023-now	**ML Infrastructure & Distributed Training**, PyTorch Distributed, JAX (pmap), CUDA, Multimodal LLMs
2023-now	**Quantum AI & Fault Tolerance**, Fault-Tolerant Quantum Computing (FTQC), Quantum Error Correction (QEC)
2024-now	**Data Pipelines & Synthetic Generation**, Large-Scale Synthetic Datasets, Vector Databases (ChromaDB)
2012-now	**Programming & HPC Operations**, Python, C++, MPI, Slurm, High-Performance Computing (HPC)
2012-now	**Rigorous Mathematical Modeling**, Phase-Space Lattice Boltzmann Method (PS-LBM), PySCF

Professional Experience

2026-now	**Founder & Chief Scientific Officer**, Point Reyes Sound, Inc. (Delaware C-Corporation)
2025-2026	**Principal Researcher**, Point Reyes Sound Research Initiative, Cupertino, CA
2024-2025	**Senior Computational Scientist, AI & Solutions**, PsiQuantum, Palo Alto, CA, USA
2023-2024	**Staff Researcher in Quantum AI**, University of Chicago, Chicago, IL, USA
2017-2023	**Postdoctoral Research Fellow (Computational Science)**, UC Berkeley & LBNL, Berkeley, CA, USA
06-08/2022	**Scientific Computing Consultant**, NewtonX, Remote, part-time, USA
2018-2020	**Scientific Software Engineer**, Q-Chem Inc., CA, USA

Education

University of California, Berkeley and Lawrence Berkeley National Laboratory — *Berkeley, CA, USA*
Postdoctoral Research Fellow in Computational Materials Science — *2017-2023*
Advisor: Prof. Martin Head-Gordon

University of Chicago — *Chicago, IL, USA*
MS, Ph.D. in Theoretical and Computational Quantum Chemistry — *2012-2017*
Advisor: Prof. David A. Mazziotti

IIT Bombay — *Bombay, India*
Master of Science — *2009-2012*
Thesis: Relativistic Quantum Mechanics of the Pionium Atom in Uniform Magnetic Fields

St Stephen's College, Delhi — *Delhi, India*
B.Sc (Hons) in Chemistry, with Physics and Mathematics — *2006-2009*

Point Reyes Sound, Inc. — *San Francisco, CA*
Founder & Principal Researcher — *Mar 2025 -- Present*

- **FTQC Resource Compilation Brief:** Engineered a classical-to-quantum active-space compiler and block-encoded qubitization pipeline, publishing exact resource bounds (1.66×10^9 T-gates, 168 logical qubits on Cr_2) to prove a 1,747x reduction in Toffoli gate complexity against full-system FTQC benchmarks.
- **Hardware Adaptation & SRAM Streaming:** Mapped the Quantum Boltzmann Equation (QBE-SCF) framework to Apple Silicon's Tile-Based Deferred Rendering (TBDR) pipeline, bypassing memory bandwidth walls via 32 KB on-chip SRAM tile streaming to achieve a >3.0x asymptotic speedup over CPU cache-throttled baselines while maintaining microhartree accuracy.
- **AI-Accelerated Phase-Space Transport:** Developed a Hessian-free orbital optimization framework utilizing continuous phase-space fluid advection and the BGK collision operator to autonomously offload dynamic correlation via differentiable JAX kernels.
- **Intellectual Property & Commercialization:** Authored, filed, and formally assigned U.S. Provisional Patent App. No. 64/033,274 (Quantum Boltzmann Equation framework) to commercialize quantum-accelerated electronic structure solvers for partner integration.

PsiQuantum, Corp. *Palo Alto, CA*
Senior Computational Scientist, Quantum Solutions *Oct 2024 -- Mar 2025*

- **Partner Workload Translation:** Engineered scalable distributed simulation pipelines, translating complex quantum mechanical domain problems into performant, production-ready software for cross-functional benchmarking.

University of Chicago *Chicago, IL*
Staff Researcher, Generative AI & Machine Learning *Nov 2023 -- Oct 2024*

- **Domain Adaptation for Generative AI (Azure Grant):** Secured the Microsoft Azure Accelerate Foundation Models Research grant to pioneer the integration of physical symmetries into generative architectures (PyTorch/JAX), establishing exact structural equivalence benchmarks to evaluate OOD mode collapse in partner-relevant domains.
- **Physics-Grounded Generative Workflows (NeurIPS 2026):** Led the development of a symmetry-aware framework conditioning generative outputs on strict physical constraints (geometry, charge/spin, point-group symmetry), effectively solving out-of-distribution mode collapse.
- **Automated Evaluation & Distributed Training (JCTC 2026):** Built distributed training pipelines natively in PyTorch to generate mathematically-verified synthetic supervision data, establishing evaluation metrics defined by exact structural equivalences rather than heuristics.

Publications

$^{+}$ *Equal Contributors*

In Preparation & Submitted

Chakraborty, R. Hardware Resource Compilation for Active-Space Driven Fault-Tolerant Quantum Simulation, *Technical Brief / In Preparation for PRX Quantum,* ***2026***.

Chakraborty, R. Rendering the Quantum Fluid: Mapping Phase-Space Electronic Structure to Tile-Based Deferred Shading, *Technical Brief, Point Reyes Sound, Inc.,* ***2026***.

Chakraborty, R. Quantum Boltzmann Equation Self-Consistent-Field Method for Entropic Regularization of Mean-Field Singularities near Conical Intersections, *Submitted to The Journal of Chemical Physics,* ***2026***.

Chakraborty, R. The Quantum Boltzmann Entrainment Tensor: A Hessian-Free Framework for Multireference Orbital Optimization, *In Preparation for JCTC,* ***2026***.

Chakraborty, R. Crystalline Phase-Space Lattice Boltzmann Method: k-Space Generalization of Entropic Regularization in Periodic Solids, *In Preparation for Physical Review Letters,* ***2026***.

Chakraborty, R. Hardware Resource Compilation for Active-Space Driven Fault-Tolerant Quantum Simulation, *In Preparation for PRX Quantum,* ***2026***.

Chakraborty, R. On the Kinetic Origin of the CO dipole moment, *In Preparation,* ***2026***.

Chakraborty, R. Phase-Space Tomography Reveals Hidden Topology in Chemical Bonding, *In Preparation for Nature Chemistry,* ***2026***.

In Print

Chakraborty, R., Talbot, J. J., Shen, H., Yabuuchi, Y., Jiang, H., Carsch, K.M., Furukawa, H., Long, J.R., Head-Gordon, M. ***2024***. Quantum Chemical Modeling of Hydrogen Binding in Metal-Organic Frameworks: Validation, Insight, Predictions and Challenges. *Selected as a Hot Article*. Phys. Chem. Chem. Phys. 26 (8), 6490-6511

Carsch, K.M.,**Chakraborty, R.**, Head-Gordon, M, Long, J.R. et. al. . ***2023***. Selective Adsorption of Oxygen from Humid Air in a Metal–Organic Framework with Trigonal Pyramidal Copper(I) Sites. J. Am. Chem. Soc. 2024, 146, 5, 3160–3170

Talbot J.J., **Chakraborty, R.**, Shen, H., Head-Gordon, M. ***2023***. A Free Energy Decomposition Analysis: Insight into Binding Thermodynamics from Absolutely Localized Molecular Orbitals. *J. Phys. Chem. Lett.*, 14, 5432-5440.

Funke L.M., **Chakraborty R.**, Carsch, K.M., Head-Gordon, M., Long, J.R., Reimer, J.A..***2023***. Assessment of Adsorbate π-backbonding in Cu(I) Metal–Organic Frameworks via Multinuclear NMR Spectroscopy and Density Functional Theory Calculations. *J. Phys. Chem. C* 127 (15): 7513–7519

Chakraborty, R., Carsch, K.M., Jaramillo, David E, Yabuuchi Tuto, Furukawa H, Long, J.R., Head-Gordon M. ***2022***. Prediction of Multiple Hydrogen Ligation at a Vanadium(II) Site in a Metal-Organic Framework. *J. Phys. Chem. Lett.*, 13(44): 10471-10478.

Barnett, B.R., Evans, H.A, Su, G.M., Jiang, H.Z.H., **Chakraborty, R.**, Banyeretse, D., Hartman, T.J., Martinez, M.B., Trump, B.A., Tarver, J.D., Dods, M.N., Funke, L.M., Borgel, J., Reimer, J.A., Drisdell, W.A., Hurst, K.E., Gennett, T., FitzGerald, S.A., Brown, C.M., Head-Gordon, M., Long, J.R. ***2021***. Observation of an Intermediate to H2 Binding in a Metal–Organic Framework. 2021. *J. Am. Chem. Soc.*, 143(36): 14884-14894.

Epifanovsky E., Gilbert A.T.B., Feng X., Lee J., Mao Y., Mardirossian N., ..., **Chakraborty, R.**, ..., Head-Gordon, M., Herbert J.M., Krylov, A.I. Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. ***2021***. *J. Chem. Phys.*, 155(8):084801

Jaramillo, D.E., Jiang, H.Z.H., Evans, H.A., **Chakraborty, R.**, Furukawa, H., Brown, C.M., Head-Gordon, M., Long, J.R. ***2021***. Ambient-temperature hydrogen storage via vanadium (II)-dihydrogen complexation in a metal–organic framework. *J. Am. Chem. Soc.*, 143(16):6248:6256

Stauch T.$^{+}$, **Chakraborty, R.**$^{+}$, Head-Gordon, M. 2019. Quantum Chemical Modeling of Pressure Induced Spin Crossover in Octahedral Metal Ligand Complexes. ***2019***. *ChemPhysChem*, 20(21):2742-2747

Chakraborty, R., Mazziotti, D.A. ***2018***. Sparsity of the wavefunction from the generalized Pauli exclusion principle. *J. Chem. Phys.* 148 (5), 054106.

Chakraborty, R., Mazziotti, D.A. 2017. Noise-assisted energy transfer from the dilation of the set of one electron reduced density matrices. ***2017***. *J. Chem. Phys.* 146 (18), 184101.

Chakraborty, R., Mazziotti, D.A. ***2016***. Role of the generalized Pauli constraints in the quantum chemistry of excited states. *Int. J. Quantum Chem.* 116 (10), 784-790.

Chakraborty, R., Mazziotti, D.A. ***2015***. Structure of the one electron reduced density matrix from the generalized Pauli exclusion principle. *Int. J. Quantum Chem.* 115 (19), 1305-1310.

Chakraborty, R., Mazziotti, D.A. ***2015***. Sufficient condition for the openness of a many electron quantum system from the violation of a generalized Pauli exclusion principle. *Physical Review A* 91 (1), 010101

Datta, S. N., Ghosh A., **Chakraborty, R.**. ***2015***. Variational aspects of the Klein–Gordon equation. *Ind. J. Phys.* 89 (2), 181-187.

Chakraborty, R., Mazziotti, D.A. ***2014***. Generalized Pauli conditions on the spectra of one electron reduced density matrices of atoms and molecules. *Phy. Rev. A* 89 (4), 042505.

`https://scholar.google.com/citations?hl=en&user=m4HlFRIAAAAJ&view_op=list_works&sortby=pubdate`

Awards, Fellowships, & Grants

Fall, 2023	**Accelerate Foundation Models Research**, Microsoft Research for fine-tuning OpenAI models
Smr, 2023	**Award for Contributions to Inclusion in Science and Society**, Berkeley Lab (Postdoc Assoc.)
Smr, 2023	**Successful EOI for Independent Early Career Fellowships**, University of Oxford, UK
Fall, 2015	**Arts Science and Culture Graduate Fellowship**, University of Chicago, USA
Smr, 2009	**Lindau Graduate Fellowship**, German Research Foundation (DFG)

Outreach & Professional Development

Peer Review

Nature Communications, 2022
Journal of Chemical Theory and Computation, 2023
Molecular Physics, 2018, 2019, 2020
Journal of Physics: Condensed Matter, 2017

Professional Memberships

American Physical Society
Councillor (alternate) at California Section of the American Chemical Society (2023-2026) Program Book Coordinator at the Western Regional Meeting (2025)
Project SEED (Summer Opportunities for Economically Disadvantaged Students) (2025-2026)