

Romit Chakraborty

☎ +1 773-816-8338 | ✉ romit@pointreysound.com | 🏠 rchakraborty.dev | 🌐 www.pointreysound.com

Profile

Quantum chemist and architect of phase-space electronic structure theory. My research develops Quantum Boltzmann Equation (QBE) solvers that regularize mean-field singularities and scale the exponential walls of strongly correlated quantum matter. Building on postdoctoral research at UC Berkeley and doctoral training at the University of Chicago, I now direct Point Reyes Sound, Inc.

Skills

2012--now	HPC	Python, C++, MPI, Slurm, GPU Acceleration, Linux
2012--now	Quantum Simulation	FTQC, QEC, Quantum Boltzmann Equation (QBE)
2022--now	Data Pipelines	Vector Databases, ChromaDB, Azure
2023--now	ML Infrastructure	PyTorch, JAX, LLMs, LoRA

Education

University of Chicago	<i>Chicago, IL, USA</i>
MS, PH.D. IN THEORETICAL AND COMPUTATIONAL QUANTUM CHEMISTRY	<i>2012--2017</i>
Advisor: Prof. David A. Mazziotti	
IIT Bombay	<i>Mumbai, India</i>
MASTER OF SCIENCE IN CHEMISTRY	<i>2009--2012</i>
St. Stephen's College, University of Delhi	<i>Delhi, India</i>
B.Sc. (HONS) IN CHEMISTRY, WITH PHYSICS AND MATHEMATICS	<i>2006--2009</i>

Research Experience

Point Reyes Sound, Inc.	<i>San Francisco, CA</i>
FOUNDER & CEO	<i>June 2026 -- Present</i>
• Phase-Space Electronic Structure: Formulated a Hessian-free orbital optimization framework utilizing continuous phase-space fluid advection and the Bhatnagar-Gross-Krook (BGK) collision operator to autonomously regularize mean-field singularities. • Quantum Boltzmann Entrainment Tensor (QBET): Developed a framework coupling classical phase-space relaxation to an active-space quantum core, circumventing combinatorial active-space expansion and demonstrating monotonic CASSCF orbital convergence on multireference dissociation benchmarks up to 254-orbital basis sets. • Solid-State k-Space Decoupling: Generalized the phase-space transport engine for periodic crystalline systems by projecting continuous Wigner distributions onto cGTOs, mapping multidimensional transport to decoupled matrix relaxations across the Brillouin zone.	
PsiQuantum, Corp.	<i>Palo Alto, CA</i>
SENIOR QUANTUM SOLUTIONS CHEMIST	<i>Oct 2024 -- Mar 2025</i>
• Translated quantum chemical models of correlated electron systems into algorithmic compilation pipelines and active-space resource estimation frameworks for fault-tolerant quantum hardware architectures.	

University of Chicago

STAFF RESEARCHER IN QUANTUM AI

Chicago, IL

Nov 2023 -- Oct 2024

- **Physics-Grounded Generative Workflows:** Led the development of an equivariant framework conditioning generative models on exact physical invariants (molecular geometry, charge/spin multiplicity, point-group symmetry) to mitigate out-of-distribution mode collapse.
- **Physical Symmetry Integration:** Integrated point-group and rotational symmetries into multimodal foundation models, securing Microsoft Azure Accelerate Foundation Models Research funding for automated quantum chemical discovery.
- **Structural Verification Metrics:** Designed deterministic validation protocols for synthetic molecular configurations, evaluating model fidelity against exact graph automorphisms and quantum chemical invariant sets rather than heuristic approximations.

University of California, Berkeley & Lawrence Berkeley National Laboratory

POSTDOCTORAL RESEARCH FELLOW

Berkeley, CA

2017 -- 2023

- **MOF Chemistry:** Modeled dihydrogen binding and multi-ligand coordination at open metal sites (V(II), Cu(I)) in metal-organic frameworks under Prof. Martin Head-Gordon, validating predictions against experimental neutron scattering and adsorption isotherms (JACS, PCCP Hot Article).
- **Free Energy Decomposition:** Formulated an Absolutely Localized Molecular Orbital Free Energy Decomposition Analysis (ALMO-FEDA) to resolve vibrational and entropic driving forces in non-covalent binding thermodynamics (J. Phys. Chem. Lett.).
- **Quantum Chemistry Software:** Co-developed modular quantum chemistry capabilities for open-shell and correlated electronic structure as a code contributor to the open-source Q-Chem 5 package (J. Chem. Phys.).

Publications

⁺ *Equal Contributors*

PREPRINTS

1. **Chakraborty, R.** (2026). [Quantum Boltzmann Equation Self-Consistent-Field for the Entropic Regularization of Mean-Field Singularities](#). *arXiv:2608.14979 [quant-ph, physics.chem-ph]*. [arXiv:2608.14979] [PDF]

PEER-REVIEWED JOURNAL ARTICLES

1. **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. *Phys. Chem. Chem. Phys.*, 26(8), 6490--6511. (*Selected as PCCP Hot Article*).
2. Carsch, K. M., **Chakraborty, R.**, Head-Gordon, M., Long, J. R., et al. (2024). Selective Adsorption of Oxygen from Humid Air in a Metal-Organic Framework with Trigonal Pyramidal Copper(I) Sites. *J. Am. Chem. Soc.*, 146(5), 3160--3170.
3. 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(24), 5432--5440.
4. 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.
5. **Chakraborty, R.**, Carsch, K. M., Jaramillo, D. E., Yabuuchi, Y., 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.
6. 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. *J. Am. Chem. Soc.*, 143(36), 14884--14894.

7. 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. (2021). Software for the Frontiers of Quantum Chemistry: An Overview of Developments in the Q-Chem 5 Package. *J. Chem. Phys.*, 155(8), 084801.
8. 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.
9. Stauch, T.⁺, **Chakraborty, R.**⁺, Head-Gordon, M. (2019). Quantum Chemical Modeling of Pressure Induced Spin Crossover in Octahedral Metal Ligand Complexes. *ChemPhysChem*, 20(21), 2742--2747.
10. **Chakraborty, R.**, Mazziotti, D. A. (2018). Sparsity of the Wavefunction from the Generalized Pauli Exclusion Principle. *J. Chem. Phys.*, 148(5), 054106.
11. **Chakraborty, R.**, Mazziotti, D. A. (2017). Noise-Assisted Energy Transfer from the Dilation of the Set of One-Electron Reduced Density Matrices. *J. Chem. Phys.*, 146(18), 184101.
12. **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.
13. **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.
14. **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. *Phys. Rev. A*, 91(1), 010101.
15. Datta, S. N., Ghosh, A., **Chakraborty, R.** (2015). Variational Aspects of the Klein-Gordon Equation. *Indian J. Phys.*, 89(2), 181--187.
16. **Chakraborty, R.**, Mazziotti, D. A. (2014). Generalized Pauli Conditions on the Spectra of One-Electron Reduced Density Matrices of Atoms and Molecules. *Phys. Rev. A*, 89(4), 042505.

TECHNICAL REPORTS & WHITEPAPERS

1. **Rendering the Quantum Fluid: Mapping Phase-Space Electronic Structure to Tile-Based Deferred Shading**, *Point Reyes Sound Technical Whitepaper PRS-TR-2026-02, 2026*. [PDF] [Interactive Dossier]
2. **The Quantum Boltzmann Entrainment Tensor: A Hessian-Free Framework for Multireference Orbital Optimization**, *Point Reyes Sound Technical Report PRS-TR-2026-01 / In Preparation for JCTC, 2026*. [PDF] [Interactive Dossier]
3. **Quantum Resource Estimation: Hardware Resource Compilation for Active-Space Driven Fault-Tolerant Quantum Simulation**, *Point Reyes Sound Technical Whitepaper PRS-TR-2026-03, 2026*. [PDF]

[Link to Google Scholar Profile ↗](#)

Awards

- Fall, 2023 **Accelerate Foundation Models Research**, Microsoft Azure
Snr, 2023 **Award for Contributions to Inclusion in Science and Society**, Berkeley Lab
Snr, 2023 **EOI for Independent Early Career Fellowships**, University of Oxford, UK
Fall, 2015 **Arts Science and Culture Graduate Fellowship**, University of Chicago, USA
Snr, 2009 **Lindau Graduate Fellowship**, German Research Foundation (DFG)

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 (October 2025)

Project SEED (Summer Opportunities for Economically Disadvantaged Students) (2025-2026)

Member at Large, Cal ACS 2026-2027

