Rishab Dutta

Homepage LinkedIn GitHub Google Scholar rishab.dutta@yale.edu

Experience

Yale University

Postdoctoral Associate, Department of Chemistry (Fall 2023 – present)
Advisor: Prof. Victor S. Batista

Education

Rice University

Ph.D. in Chemistry (2023)
Advisor: Prof. Gustavo E. Scuseria

Rice University

M.A. in Chemistry (2019)
CPI: 3.94/4.00

Indian Institute of Technology Bombay

M.Sc. in Chemistry (2017)
CPI: 9.12/10.00

University of Calcutta

B.Sc. in Chemistry with Physics and Mathematics (2015)
Honours in Chemistry with first class

Publications

3. Armin Khamoshi, **Rishab Dutta**, Gustavo E. Scuseria. State preparation of antisymmetrized geminal power on a quantum computer without number projection. *J. Phys. Chem. A* (2023) preprint article
2. **Rishab Dutta**, Guo P. Chen, Thomas M. Henderson, Gustavo E. Scuseria. Construction of linearly independent non-orthogonal AGP states. *J. Chem. Phys.* **154**, 114112 (2021) preprint article
1. **Rishab Dutta**, Thomas M. Henderson, Gustavo E. Scuseria. Geminal replacement models based on AGP. *J. Chem. Theory Comput.* **16**, 6358 (2020) preprint article

Research Interests

- Understanding interesting quantum systems
- Quantum methods implementable in classical and quantum computers
- Algebra emerging from many-body quantum mechanics
- Tensor networks, decompositions, and symmetries

Awards

- *Fall Travel Award*, Chemistry Graduate Student Association, Rice University, USA (2022)
- *Harry B. Weiser Research Award*, Department of Chemistry, Rice University, USA (2021)
- *Summer Research Programme Bursary*, School of Chemistry, University of Birmingham, UK (2016)
- *INSPIRE Scholarship for Higher Education*, Department of Science and Technology, Government of India (2012 – 2017)

Achievements

- Research featured in *Enquiry Magazine*, Winter issue, Rice University (2022)
- Selected for the *Sci-Mix Presentations*, ACS Fall National Meeting, American Chemical Society (2022)
- *All India Rank 57* among around 40000 candidates, National Eligibility Test for Chemical Sciences, Council of Scientific and Industrial Research and University Grants Commission (2015)
- *All India Rank 15* among around 7000 candidates, Joint Admission Test for Chemistry, Indian Institute of Science and Indian Institutes of Technology (2015)

Selected Past Research

Rice University

Ph.D. candidate at the Department of Chemistry (Summer 2019 – Summer 2023).

- Development of methods based on correlated pairs for strong electron correlation
- Application to model paired fermionic and spin one-half systems
- Development of quantum state preparation algorithms

Rice University

Graduate student researcher at the Department of Chemistry (Fall 2017 – Spring 2019).

- Development of variants of coupled cluster methods for strong electron correlation
- Application to model fermionic Hamiltonians and molecular dissociations

Teaching Experience

CHEM 531: Advanced Quantum Chemistry

Teaching assistant at Rice University (Spring 2021, Spring 2022, Spring 2023)

- Presented tutorials on using the Gaussian software
- Helped students with their assignments during the lab sections
- Designed and graded assignments

CHEM 430/530: Quantum Chemistry

Teaching assistant at Rice University (Fall 2021, Fall 2022)

- Helped students with their assignments and concepts during the office hours
- Designed and graded course assignments and exams
- Prepared and presented lectures on *Symmetry and Spectroscopy*

CHEM 124: General Chemistry Lab II

Teaching assistant at Rice University (Spring 2018)

- Helped students with their experiments during the lab sections
- Graded assignments

CHEM 123: General Chemistry Lab I

Teaching assistant at Rice University (Fall 2017, Fall 2018)

- Helped students with their experiments during the lab sections
- Graded assignments

Talks

- *ACS Fall National Meeting*, American Chemical Society, Chicago (August, 2022)
- *CHEM 600: Physical Chemistry*, Rice University, Houston (Spring 2018, Fall 2018, Spring 2020, Fall 2020, Fall 2021, Fall 2022)

Posters

- *Frontiers in Computational Chemistry: The NYU Simons Center Inaugural Symposium*, New York University and Simons Center, New York City (October, 2022)
- *Sci-Mix Presentations at the ACS Fall National Meeting*, American Chemical Society, Chicago (August, 2022)
- *10th Triennial Conference on Molecular Quantum Mechanics*, Virginia Tech, Blacksburg (June, 2022)
- *Workshop on HPC in Computational Chemistry and Materials Science*, Molecular Sciences Software Institute, virtual (December, 2021)
- *The 7th Annual SCI Summer Research Colloquium*, Smalley-Curl Institute, Houston (August, 2021)

Workshops

- *Qiskit Global Summer School on Quantum Simulation*, Qiskit and IBM, virtual (July, 2022)
- *ComSciCon-Houston*, ComSciCon, Houston (March, 2022)
- *Telluride School on Theoretical Chemistry*, Telluride Science Research Center, virtual (July, 2021)
- *Qiskit Global Summer School on Quantum Machine Learning*, Qiskit and IBM, virtual (July, 2021)
- *Introduction to Quantum Computing*, The Coding School and IBM, virtual (Fall 2020 – Spring 2021)

Skills

Coding

- Fortran
- Julia
- Python

Writing

- LaTeX
- Vim
- Markdown
- HTML

Software

- Git
- Jupyter Notebook
- Gaussian

Languages

- Bengali (native proficiency)
- English (full professional proficiency)
- Hindi (professional working proficiency)

Programming Experience

- Algorithms for quantum chemistry research
- Linear algebra and matrix computations
- Non-linear multi-dimensional optimizations
- Tensor contractions and decompositions

Interests

- Science Communicator, personal blog (2017 – present)
- Contributing Writer, *Enquiry Magazine*, Wiess School of Natural Sciences, Rice University (2021 – 2022)
- Contributor, Bengali translation of *Qiskit* documentation (2021 – 2022)
- Volunteer, international orientation events organized by the Office of International Students & Scholars, Rice University (2019 – 2021)