Curriculum Vitae

Arnab Chakraborty

Graduate Assistant, MSUID: A58275463
Department of Chemistry, Michigan State University
Chemistry Building, 578 S. Shaw Lane, Room 18A
East Lansing, Michigan, 48824-1322, U.S.A.
Telephone: (517) 353-1154
Email: chakra56@chemistry.msu.edu

EDUCATION

Michigan State University | U.S.A. (August 2018 – present)

- Pursuing Ph.D. in Theoretical and Computational Chemistry
- Advisor: Professor Piotr Piecuch

Indian Institute of Technology Kanpur | India (July 2016 – June 2018)

- M.Sc. in Chemistry
- Advisor: Dr. Madhav Ranganathan

University of Calcutta | India (August 2013 – May 2016)

- B.Sc. in Chemistry (Honours)

PROFESSIONAL EXPERIENCE

Michigan State University | U.S.A. (August 2018 – present)
Graduate Research Assistant and Teaching Assistant. Teaching freshmen-level general chemistry (CEM 141), senior level statistical mechanics (CEM 484), and physical chemistry laboratory (CEM 395 and CEM 495) courses, while performing Ph.D. research in theoretical and computational chemistry. Advisor: Professor Piotr Piecuch.

Indian Association for the Cultivation of Science | India (May 2017 – July 2017)
Summer Project Student. Advisor: Professor Satrajit Adhikari.

University of Calcutta | India (May 2016 – June 2016)
Summer Project Student. Advisor: Professor Pinaki Chaudhury.

RESEARCH EXPERIENCE

Michigan State University | U.S.A. (August 2018 – present)
Graduate Student Researcher. Advisor: Professor Piotr Piecuch.

- I am currently working on the development and applications of novel coupled-cluster (CC) methods and their excited-state equation-of-motion (EOM) extensions suitable for studying open-shell systems, especially radicals and biradicals. In particular, I am developing semi-stochastic versions of the electron-attachment (EA) and ionization-potential (IP) EOMCC

approaches and their double electron-attachment (DEA) and double ionization-potential (DIP) counterparts capable of converging target high-level EA/IP and DEA/DIP EOMCC energetics out of the early stages of Quantum Monte Carlo (QMC) propagations in the many-electron Hilbert space. I am also working toward extending the non-iterative energy corrections defining the CC/EOMCC methodology abbreviated as CC(*P*;*Q*) to the particle non-conserving EA/IP and DEA/DIP regimes.

- I have been involved in a collaborative effort with other members of the Piecuch group aimed at combining the deterministic CC(*P*;*Q*) methodology for excited electronic states with the stochastic QMC approaches to recover high-level EOMCC (e.g., EOMCCSDT) energetics in the early stages of QMC propagations. I have also worked on assessing the performance of the QMC-driven CC(*P*;*Q*) methods in calculations of singlet–triplet gaps in organic biradicals.
- I have been involved in a larger collaborative project involving our group and the groups of Professors Gary Blanchard, Babak Borhan, Marcos Dantus, James Jackson, and Ehud Pines aimed at the fundamental understanding of the behavior and properties of a novel super photobase discovered in our department designated as **FR0**-SB, which exhibits a change in pK_a by about 14 units and deprotonates alcohols in a solution upon photoexcitation, as well as its singly and doubly protonated forms.
- I have also been involved in a collaboration between our group and the group of Professor Marcos Dantus focusing on experimental and theoretical studies of chemical reaction dynamics resulting from strong-field double ionization of small organic molecular species in the gas phase.

Indian Institute of Technology Kanpur | India (July 2016 – June 2018)
Advisor: Dr. Madhav Ranganathan.

- I calculated surface stress in the (001) plane of silicon during different reconstructions using density functional theory.

Indian Association for the Cultivation of Science | India (May 2017 – July 2017)
Summer Project Advisor: Professor Satrajit Adhikari.

- I studied the dynamic Jahn–Teller effect in octahedrally coordinated d^9 Cu cations. I wrote a computer code that solves the Mathieu differential equation, needed to study the dynamic Jahn–Teller effect, numerically.

University of Calcutta | India (May 2016 – June 2016)
Summer Project Advisor: Professor Pinaki Chaudhury.

- I conducted a literature survey regarding the structures of endohedral metallofullerenes.

SOFTWARE SKILLS

Scientific Programming: Fortran, Python, Julia
Computational Software: GAMESS, NWChem, PySCF, HANDE, NECI, Quantum Espresso

AWARDS

DST-INSPIRE Scholarship for Higher Education (2013 – 2018) for being within the top 1% of my

Class XII Examination of my State Board (West Bengal Council of Higher Secondary Education).

PUBLICATIONS*

1. S.H. Yuwono, **A. Chakraborty**, J.E. Deustua, J. Shen, and P. Piecuch, "Accelerating Convergence of Equation-of-Motion Coupled-Cluster Computations Using the Semi-Stochastic CC(*P*;*Q*) Formalism", *Mol. Phys.* **118**, e1817592 (2020) (17 pages) [Special Issue in Honour of Professor Jürgen Gauss; invited contribution]. This article was selected by the Editors of *Molecular Physics* as the best paper published in the journal in the year 2020.

2. **A. Chakraborty**, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Benchmarking the Semi-Stochastic CC(*P*;*Q*) Approach for Singlet–Triplet Gaps in Biradicals", *J. Chem. Phys.* **157**, 134101 (2022).

3. **A. Chakraborty**, S. Basumallick, J. Shen, and P. Piecuch, "Extension of the Semi-Stochastic Equation-of-Motion Coupled-Cluster Formalism to the Single and Double Electron Attachment and Ionization Potential Schemes", manuscript in preparation for *J. Phys. Chem. A*.

*Clickable hyperlinks to published papers are marked by blue color.

TALKS AND POSTERS

1. **A. Chakraborty**, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Benchmarking the Semi-Stochastic CC(*P*;*Q*) Approach for Singlet–Triplet Gaps in Biradicals", *Conference Talk*, 52nd Midwest Theoretical Chemistry Conference (MWTCC), June 2–4, 2022, The Ohio State University, Columbus, Ohio, U.S.A.

2. **A. Chakraborty**, J. Shen, and P. Piecuch, "Quantum-Monte-Carlo-Driven Equation-of-Motion Coupled-Cluster Approaches for Electron Attachment and Ionization: Implementation and Applications", *Conference Poster*, 52nd Midwest Theoretical Chemistry Conference (MWTCC), June 2–4, 2022, The Ohio State University, Columbus, Ohio, U.S.A.

3. **A. Chakraborty**, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Applications of the Semi-Stochastic CC(*P*;*Q*) Approach for Calculating Singlet–Triplet Gaps in Biradical Systems", *Conference Poster*, The 2020 American Conference on Theoretical Chemistry (ACTC 2020), Palisades Tahoe (formerly Squaw Valley), California, U.S.A., July 26-30, 2020. DUE TO COVID-19, RESCHEDULED TO July 24-28, 2022; renamed ACTC 2022.

4. **A. Chakraborty**, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Exploring Electronic Excitations in Molecules and Singlet–Triplet Gaps in Biradicals: A Semi-Stochastic CC(*P*;*Q*) Study", *Conference Poster*, 53nd Midwest Theoretical Chemistry Conference (MWTCC), June 1–2, 2023, Purdue University, West Lafayette, Indiana, U.S.A.

5. **A. Chakraborty**, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Application of the Semi-Stochastic CC(*P*;*Q*) Approach for Electronic Excitations in Molecules and Singlet–Triplet Gaps in Biradicals", *Invited Talk*, The symposium "Computational Chemistry From Electrons to Macromolecules," the 2023 Central Regional Meeting of the American Chemical Society (CERM 2023), Dearborn, Michigan, U.S.A., June 20-23, 2023.

TALKS AND POSTERS AT CONFERENCES PRESENTED BY CO-AUTHORS

1. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and **A. Chakraborty**, "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, Utah, U.S.A., September 22–27, 2019 [invited talk given by P. Piecuch].

2. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and **A. Chakraborty**, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Workshop on New Methods for Strongly Correlated Electrons, Qingdao, China, October 9–13, 2019 [invited talk given by P. Piecuch].

3. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and **A. Chakraborty**, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The international conference "Quantum International Frontiers 2019," Shanghai, China, November 18–22, 2019 [invited Frontier Lecture given by P. Piecuch].

4. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and **A. Chakraborty**, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," the 60th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 16–21, 2020 [invited talk given by P. Piecuch].

5. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, and K. Gururangan, "High-Accuracy Electronic Energetics by Stochastic and Deterministic Wave Function Sampling and Coupled-Cluster Computations," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2020), 5th edition, Telluride, Colorado, U.S.A., June 1-5, 2020. DUE TO COVID-19, REPLACED BY VIRTUAL WORKSHOP, June 1–5 and June 8–9, 2020 [invited talk given by P. Piecuch via Zoom].

6. P. Piecuch, J. Shen, J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, and K. Gururangan, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," TSRC Workshop "New Frontiers in Electron Correlation," 3rd edition, Telluride, Colorado, U.S.A., June 14–18, 2021 [virtual workshop; invited talk given by P. Piecuch via Zoom].

7. P. Piecuch, J. Shen, J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, and K. Gururangan, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," TSRC Workshop "New Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 19-23, 2021 [hybrid format; invited talk given by P. Piecuch via Zoom].

8. P. Piecuch, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations", with contributions from J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, K. Gururangan, and J. Shen, International

Symposium on Correlated Electrons (SymCorrel21), Munich Center for Quantum Science and Technology, Munich, Germany, October 5–7, 2021 [virtual workshop; invited talk given by P. Piecuch via Zoom].

9. P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected- CI-Driven Coupled-Cluster Computations," The Seventeenth Theoretical Chemistry Symposium (TCS 2021), Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia, West Bengal, India, December 11-14, 2021 [virtual symposium; invited plenary lecture given by P. Piecuch].

10. P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected- CI-Driven Coupled-Cluster Computations," Chris Cramer 60th Birthday Symposium, 263rd American Chemical Society National Meeting, San Diego, California, U.S.A., March 20–24, 2022 [hybrid symposium; pre-recorded virtual presentation; invited talk given by P. Piecuch].

11. S. Basumallick, **A. Chakraborty**, J. Shen, and P. Piecuch, "Development and Implementation of Semi-Stochastic Double Electron Attachment and Double Ionization Potential Equation-of-Motion Coupled-Cluster Approaches", Conference Poster, 52nd Midwest Theoretical Chemistry Conference (MWTCC), June 2–4, 2022, Ohio State University, Columbus, Ohio, U.S.A.

12. P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected- CI-Driven Coupled-Cluster Computations," Twelfth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, British Columbia, Canada, August 16-21, 2020 [invited talk given by P. Piecuch]. DUE TO COVID-19, RESCHEDULED TO July 3–8, 2022.

13. P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The 2020 American Conference on Theoretical Chemistry (ACTC 2020), Palisades Tahoe (formerly Squaw Valley), California, U.S.A., July 26–30, 2020 [invited talk given by P. Piecuch]. DUE TO COVID-19, RESCHEDULED TO July 24-28, 2022; renamed ACTC 2022.

14. P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, and J. Shen, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Modeling and Design of Molecular Materials 2020 (MDMM 2020) Conference, Gdańsk, Poland, September 21-24, 2020 [invited talk given by P. Piecuch]. DUE TO COVID-19, RESCHEDULED TO September 19–22, 2022; renamed MDMM 2022.

15. P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, **A. Chakraborty**, K. Gururangan, and Jun Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," International conference in the series "New Horizons in Scientific Software (NHISS 2022)" entitled "The New Collaborative Platform Goes Life," Jeju Island, South Korea, December 12–15, 2022 [hybrid format; invited talk given by P. Piecuch via Zoom].

16. J. Stamm, S. Kwon, C. Wicka, S. Priyadarsini, **A. Chakraborty**, J. Shen, P. Piecuch, and M. Dantus, "H_3^+ Formation from Methyl Halogens and Pseudohalogens," 54th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, Spokane, Washington, U.S.A., June 5–9, 2023 [contributed talk to be given by J. Stamm].

17. P. Piecuch, J.E. Deustua, K. Gururangan, **A. Chakraborty**, S.H. Yuwono, S. Priyadarsini, and J. Shen, "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(*P*;*Q*) Approaches," 17th International Congress of Quantum Chemistry, Bratislava, Slovakia, June 21–26, 2021 [invited talk to be given by P. Piecuch]. DUE TO COVID-19, RESCHEDULED TO June 20-23, 2023.

18. J. Stamm, S. Kwon, C. Wicka, **A. Chakraborty**, S. Priyadarsini, J. Shen, P. Piecuch, and M. Dantus, "H_3^+ Formation from CH_3X for X = Halogens and Pseudo Halogens," The 15th Femtochemistry Conference (FEMTO 15), Berlin, Germany, July 30–August 4, 2023 [contributed talk or poster to be presented by M. Dantus].

19. P. Piecuch, J.E. Deustua, K. Gururangan, **A. Chakraborty**, S.H. Yuwono, S. Priyadarsini, and Jun Shen, "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(*P*;*Q*) Approaches," The 5th Conference on Theory and Applications of Computational Chemistry (TACC 2020), Sapporo, Japan, September 7–12, 2020 [invited talk to be given by P. Piecuch]. DUE TO COVID-19, RESCHEDULED TO June 26–July 1, 2023.