ARNAB CHAKRABORTY

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EDUCATION

Ph.D. in Theoretical and Computational Chemistry **2018 – Present**
Michigan State University, East Lansing, USA
GPA : 4.0/4.0
Advisor: Professor Piotr Piecuch

M.Sc. in Chemistry **2016 – 2018**
Indian Institute of Technology Kanpur, Kanpur, India
CGPA: 9.3/10.0
Advisor: Dr. Madhav Ranganathan

B.Sc. in Chemistry (Honours) **2013 – 2016**
University of Calcutta, Kolkata, India
Grade: 1st Division, 75%

PROFESSIONAL EXPERIENCE

Michigan State University **August 2018 – Present**

- Quantum Chemistry method development in the area of Coupled-Cluster theory with experience in developing sophisticated and efficient computer programs for numerically solving the Schrödinger equation approximately in various situations.
- Achieved significant experience working with Fortran and Python High Performance and parallel computing using OpenMP and MPI and basic experience with Julia, C/C++, and CUDA C/C++.
- Significant experience in using density functional theory (DFT) to optimize structures and calculate different properties of chemicals.
- Taught general chemistry (CEM141) to freshmen-level undergraduate students, senior level statistical mechanics (CEM484), and senior-level physical chemistry laboratory (CEM395 and CEM495) courses.

Indian Institute of Technology Kanpur **July 2016 – June 2018**

- Significant experience studying materials, especially semiconductors, using density functional theory (DFT).
- Experience in using classical molecular dynamics (MD) using AMBER to calculate different chemical properties.

Indian Association for the Cultivation of Science **May 2017 – July 2017**
Summer Project Student under Professor Satrajit Adhikari
Studied Jahn–Teller distortions in d^9 Cu cations.

University of Calcutta **May 2016 – June 2016**
Summer Project Student under Professor Pinaki Chaudhuri
Studied endohedral metallofullerenes.

RESEARCH EXPERIENCE

Michigan State University, U.S.A. **August 2018 – Present**

Graduate 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 also recently started combining classical molecular dynamics simulations with Quantum Mechanical methods in conjunction with Effective Fragment Potentials to simulate absorption and photoionization spectra of organic molecules.
- I am involved in an even larger collaborative project 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 upon photoexcitation, including its singly and doubly protonated forms.
- I have also been involved in a collaboration between our groups and several other groups focusing on experimental, high-level electronic structure, and *ab-initio* molecular dynamics simulation 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.
Performed calculations to estimate 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.
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.
Conducted a literature survey regarding the structures of endohedral metallofullerenes.

SKILLS

Scientific Programming:	Fortran/OpenMPI, Python, Julia, C/C++, CUDA C/C++
Computational Software:	GAMESS, NWChem, GROMACS, AMBER, PySCF, HANDE, NECI, QUANTUM ESPRESSO
Visualization Software:	VMD, Avogadro, MacMolPlt, Chimera
Platforms:	MS Office (Word, Excel, Powerpoint), LaTex
Analytical Techniques:	UV-Vis, IR, Raman, Fluorescence, CV, NMR, XRD

AWARDS

- Selected as one of 30 participants of the 2023 Telluride School on Theoretical Chemistry
- ACS Travel Grant from the MSU local section of ACS for my Invited talk at the 2023 Central Regional Meeting of the ACS.
- College of Natural Science Dissertation Continuation Fellowship (Summer 2022).

- 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

- 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). This article was Selected by the Editors of Molecular Physics as the best paper published in the journal in the year 2020.
- **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).
- **A. Chakraborty**, S. Basumallick, J. Shen, and P. Piecuch, " Extension of the Semi-Stochastic Equation-of-Motion (EOM) Coupled-Cluster (CC) Formalism to the Fock Space: The Single and Double Electron Attachment and Ionization Potential EOMCC Schemes", manuscript in preparation.
- J. Lahiri, E. Ben-Haimb, S.H. Yuwono, **A. Chakraborty**, D. Pines, P. Piecuch, J.E. Jackson, B. Borhan, M. Dantus, and E. Pines, "Analyzing the solvent effect on the photobasicity of FR0-SB a 'Super' Photobase", manuscript in preparation.
- J. Stamm, S. Kwon, S. Sandhu, **A. Chakraborty**, S. Priyadarsini, J. Shen, B.G. Levine, P. Piecuch, and M. Dantus, "H_3^+ Formation from Methyl Halogens and Pseudohalogens", manuscript in preparation.

INVITED TALKS AND CONFERENCE PRESENTATIONS

- **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 Ohio, U.S.A.
- **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", *Poster*, 52nd Midwest Theoretical Chemistry Conference (MWTCC), June 2–4, 2022 Ohio, U.S.A.
- **A. Chakraborty**, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Application of the Semi-Stochastic CC(P;Q) Approach for Calculating Singlet–Triplet Gaps in Biradical Systems", *Poster*, 50th American Conference on Theoretical Chemistry (ACTC), July 25–29, 2022 California, U.S.A.
- **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", *Poster*, 53nd Midwest Theoretical Chemistry Conference (MWTCC), June 1-2, 2023, Purdue University, West Lafayette, Indiana, U.S.A.
- **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.
- **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", *Poster*, 2023 Telluride School on Theoretical Chemistry, July 11–16, Telluride, Colorado, U.S.A.
- **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", *Poster*, The 41st Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference, Michigan State University, East Lansing, Michigan, U.S.A., August 1–2, 2023.

TALKS AND POSTERS PRESENTED BY CO-AUTHORS

- 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].

- 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].

- 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].

- 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].

- 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].

- 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].

- 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].

- 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].

- 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].

- 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].

- 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, 50th American Conference on Theoretical Chemistry (ACTC), July 25–29, 2022 California, U.S.A.