KARTHIK GURURANGAN

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EDUCATION

Michigan State University | East Lansing, Michigan
- Ph.D. candidate in Theoretical and Computational Chemistry
- Research Advisor: *Professor Piotr Piecuch*

Northwestern University | Evanston, Illinois
- M.S. in Materials Science
- Specialization in Integrated Computational Materials Engineering (ICME)
- Research Advisor: *Professor Elad Harel*

University of California, Berkeley | Berkeley, California
- B.S. in Materials Science and Engineering
- Minors in Physics and Mechanical Engineering
- Research Advisors: *Professor Paul K. Wright and Professor James W. Evans*

RELEVANT EXPERIENCE

Piecuch Group, Michigan State University, Dept. of Chemistry | East Lansing, MI
August 2019 – Present
Advisor: Prof. Piotr Piecuch
- Development of novel methodologies for converging high-level coupled-cluster ground- and excited-state energetics by adaptive and selected-configuration-interaction–driven CC(P;Q) moment expansions.
- Investigation of the externally corrected coupled-cluster (ec-CC) approaches based on extracting information from selected configuration interaction wave functions followed by subsequent moment-based corrections to account for higher-order many-electron correlation effects.
- Development and maintenance of CCpy, a research-level open-source Python software package, available on Github, that enables a wide range of conventional and unconventional coupled-cluster and equation-of-motion coupled-cluster computations with up to triple and quadruple excitations for ground and excited electronic states of molecular systems.

Materials and Microsystems Laboratories, HRL Laboratories | Malibu, CA
May 2023 – Present, until August 2023
Supervisor: Dr. Andrew Pan
- Working at HRL Laboratories (formerly known as the Hughes Research Laboratories) as a doctoral summer intern in the quantum device modeling group.
- Investigating the charge-stability phase diagram of multi-electron double- and triple-quantum dot qubit devices in the high-electron-number regime using a combination of selected configuration interaction and high-level coupled-cluster methodologies.

Citigroup, Personal Banking & Wealth Management, Global Analytics Summer Associate | New York, NY
June 2022 – August 2022
Supervisor: Mr. Mark McMurray

- Developed a data-driven credit risk model to help assess credit losses and set financing parameters associated with new merchant installment lending products to be offered at several commercial partners of Citibank, including The Home Depot, Best Buy, and Sears.

Harel Group, Northwestern University, Dept. of Chemistry | Evanston, IL
September 2017 – August 2019
Advisor: Prof. Elad Harel

- Developed statistical machine learning and optimization codes leveraging Python and Pytorch for chemometric data analysis, data cleaning, dimension reduction, and parameter extraction using large volumes of hyper-spectral data.
- Used Python and Matlab to perform numerical studies of quantum dynamics in nonlinear optical spectroscopies and developed a numerical viable protocol for quantum process tomography based on two-dimensional electronic spectroscopy (published in the *Journal of Chemical Physics*).
- Wrote numerical simulations in Matlab to interpret experimental spectroscopic data of photosynthetic bacteria complexes, resulting in publications to the *Journal of Chemical Physics Letters* and *Chemical Science*.

ICME Capstone Project, Northwestern University, Dept. of Materials Science | Evanston, IL
September 2017 – May 2018
Advisor: Prof. Gregory Olson

- Collaborated with a team of materials engineers from Medtronic to develop ways to numerically predict and extend the operation lifetime of Nitinol-based artificial heart valves.
- Used a combination of Python, Matlab, and chemical and mechanical simulation software including ThermoCalc and ABAQUS to carry out calculations to predict a novel alloy formulation and heat treatment for a long-lasting and biocompatible Nitinol heart valve.

Asta Group, UC Berkeley, Dept. of Materials Science & Engineering | Berkeley, CA
March 2017 – August 2017
Advisor: Prof. Mark Asta

- Performed high-throughput quantum mechanical density functional theory calculations using VASP to investigate the piezoelectric response and thermodynamic stability of a large collection of lead-free halide perovskite (ABX_3) compounds for use in potential device and sensor applications.
- Used Python data analysis and visualization tools to parse and manipulate the large volume of quantum chemical data to reveal trends in piezoelectric response with chemical structure.

Advanced Manufacturing for Energy Lab, UC Berkeley Dept. of Mechanical Engineering | Berkeley, CA
April 2015 – August 2017
Advisors: Prof. Paul Wright & Prof. James Evans

- Synthesized flexible polymer-based rechargeable batteries, supercapacitors, and thermoelectric generators for use in internet-of-things (IoT) sensor applications.
- Prototyped temperature-sensing devices based on these printed electronic components, resulting in two publications to the *Journal of Physics Conference Series*.
- Wrote codes in Matlab to perform numerical simulations of the supercapacitor operation, including using optimization algorithms to investigate the most power-efficient charging and recharging schedule.

Publications

1). K. Gururangan and P. Piecuch, "Converging High-Level Coupled-Cluster Energetics by Adaptive Selection of Excitation Manifolds Driven by Moment Expansions," *in preparation for J. Chem. Phys.*

2). S. S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "Singlet-Triplet Gap of Cyclobutadiene: The CIPSI-driven CC(*P*;*Q*) Study," *in preparation for J. Chem. Phys.*

3). M. Gordon, F. Zahariev, P. Xu, B. Westheimer, S. Webb, J.G. Vallejo, A. Tiwari, V. Sundryal, M. Sosonkina, G. Schoendorff, M. Schlinsog, T. Sattasathuchana, K. Ruedenberg, L. Roskop, A. Rendell, D. Poole, P. Piecuch, B. Pham, V. Mironov, J. Mato, S. Leonard, S. Leang, J. Ivanic, J. Hayes, T. Harville, K. Gururangan, E. Guidez, I. Gerasimov, C. Friedll, K. Ferreras, D. Federov, G. Elliot, D. Datta, D. Cruz, L. Carrington, C. Bertoni, G. Barca, and M. Alkan, "The General Atomic and Molecular Electronic Structure System (GAMESS): Novel Methods on Novel Architectures," *submitted to J. Chem. Theory Comput.*

4). K. Gururangan, J. E. Deustua, J. Shen, and P. Piecuch, "High-Level Coupled-Cluster Energetics by Merging Moment Expansions with Selected Configuration Interaction," *J. Chem. Phys.* ***155***, 174114 (2021).

5). I. Magoulas, K. Gururangan, P. Piecuch, J. E. Deustua, and J. Shen, "Is Externally Corrected Coupled Cluster Always Better Than the Underlying Truncated Configuration Interaction?,"*J. Chem. Theory Comput.* **17**, 4006 (2021).

6). S. Irgen-Gioro, K. Gururangan, A. P. Spencer, and E. Harel, "Non-Uniform Excited State Electronic-Vibrational Coupling of Pigment–Protein Complexes," *J. Phys. Chem. Lett.* **11**, 10388 (2020).

7). K. Gururangan and E Harel, "Coherent and dissipative quantum process tensor reconstructions in two-dimensional electronic spectroscopy," *J. Chem. Phys.* **150**, 164127 (2019).

8). S. Irgen-Gioro, K. Gururangan, R. Saer, R. Blankenship, and E. Harel, "Electronic coherence lifetimes of the Fenna-Mathews-Olson complex and light harvesting complex II," *Chem. Sci.* **10**, 10503 (2019).

9). Z. Gima, K. Gururangan, J. Evans, and P. Wright, "Annular screen printed thermoelectric generators for ultra-low-power sensor applications," *J. Phys. Conf. Ser.* **773**, 012115 (2016).

10). B. J. Kim, R. Winslow, I. Lin, K. Gururangan, J. Evans, and P. Wright, "Layer-by-layer fully printed Zn-MnO_2 batteries with improved internal resistance and cycle life," *J. Phys. Conf. Ser.* **660**, 012009 (2015).

PRESENTATIONS

1). 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].

2). 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].

3). 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].

4). 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].

5). 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].

6). P. Piecuch, I. Magoulas, K. Gururangan, J. E. Deustua, and J. Shen, "Externally Corrected Coupled-Cluster Methods Using Selected Configuration Interaction and FCIQMC," the 61st Sanibel Symposium, invited session on New Directions in CC Theory, St. Simons Island, Georgia, U.S.A., February 13-18, 2022
[in-person plenary lecture given by P. Piecuch]

7). 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; prerecorded virtual presentation; invited talk given by P. Piecuch].

8). P. Piecuch, I. Magoulas, K. Gururangan, J. E. Deustua, and J. Shen, "Recent Advances in Externally Corrected Coupled-Cluster Methods," 10th International Conference "Molecular Quantum Mechanics" entitled "Molecular Quantum Mechanics: Innovation, Impact, and Insight," in honor of Professors Gustavo Scuseria and Martin Head-Gordon, Blacksburg, Virginia, U.S.A., June 26 - July 1, 2022 [invited plenary lecture given by P. Piecuch].

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," Twelfth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, British Columbia, Canada, August 16-21, 2020. DUE TO COVID-19, RESCHEDULED TO July 3-8, 2022. [invited talk 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," 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. [invited talk given by P. Piecuch].

11). P. Piecuch, I. Magoulas, K. Gururangan, J. E. Deustua, and J. Shen, "Recent Advances in Externally Corrected Coupled-Cluster Methods," The symposium "Quantum Chemistry: Current and Future Frontiers," 264th American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 21-25, 2022. [in-person and virtual meeting; in-person invited talk given by P. Piecuch].

12). P. Piecuch, I. Magoulas, K. Gururangan, J. E. Deustua, and J. Shen, "Recent Advances in Externally Corrected Coupled-Cluster Methods," OPERA-2020 (Operators, Perturbations, Electrons, Relativity, and Multi-Scale Applications), an international symposium on theoretical chemistry in honor of Prof. Jürgen Gauss on the occasion of his 60th birthday, Ingelheim am Rhein, Germany, September 1-3, 2021. DUE TO COVID-19, RESCHEDULED TO August 31 - September 2, 2022. [invited talk given by P. Piecuch].

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," 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].

14). S. S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "The Singlet-Triplet Gap of Cyclobutadiene: The CIPSI-driven CC(P;Q) Study," 53rd Midwest Theoretical Chemistry Conference, Purdue University, West Lafayette, Indiana, U.S.A., June 1-3, 2023 [poster presented by S. S. Priyadarsini].

15). S. S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "Potential Energy Curves and the Singlet-Triplet Gap of Cyclobutadiene: The CIPSI-driven CC(P;Q) Study," 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 [invited talk to be given by S. S. Priyadarsini].

16). P. Piecuch, I. Magoulas, K. Gururangan, J. E. Deustua, T. Deng, and J. Shen, "Externally Corrected Coupled-Cluster Methods: Review and Recent Progress," A Satellite Symposium to the 17th International Congress of Quantum Chemistry, Znojmo, Czech Republic [invited talk to be given by P. Piecuch].

17). P. Piecuch, J. E. Deustua, K. Gururangan, A. Chakraborty, S. H. Yuwono, S. 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 26 - July 1, 2023].

18). P. Piecuch, J. E. Deustua, K. Gururangan, A. Chakraborty, S. H. Yuwono, S. S. Priyadarsini, and J. 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 September 4-9, 2023; renamed TACC 2023].

Software Skills

General and Scientific Programming: Python, Matlab, Modern Fortran, Julia
Data Science/Machine Learning: PyTorch, TensorFlow, Scikit-Learn
Simulation Software: GAMESS, NWChem, Molpro, VASP, Quantum Espresso, LAMMPS, ThermoCalc, ABAQUS

Honors and Awards

- Michigan State University, College of Natural Sciences Outstanding Student Fellowship, Summer 2023 – Awarded, but relinquished due to conflicting internship with HRL Laboratories
- U.S.A. Mathematical Olympiad (USAMO), 2012 – Participant
- American Invitational Mathematics Exam (AIME), 2012 – Top Scoring Award (14/15)
- American Mathematics Competition (AMC) 12A Examination, 2012 – High Scorer in the 99% percentile
- National Merit Scholarship Finalist, 2013
- National AP Scholar, 2013