J. Emiliano Deustua

Av. Jose de San Martin 509
Piso 2
Lima, San Bartolo 15856
Peru

Email: emiliano@examol.io
edeustua@gmail.com
Homepage: https://edeustua.xyz/
Google Scholar: 4HNQeb4AAAAJ
ORCID: 0000-0001-8193-2229

Education

- Ph.D. Chemistry, Michigan State University, 2020.
  - Dissertation Title: "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations"
  - Advisor: Piotr Piecuch
- Graduate Certificate Program High-Performance Computing, Michigan State University, 2017.
- B.S. Chemistry, Pontificia Universidad Católica del Perú, 2012.

Professional experience

- Examol Corporation, Co-founder, COO, and main engineer, 2023–present.
- Emptor, Inc., Software Engineer, 2022–2023.
- California Institute of Technology, Division of Chemistry and Chemical Engineering, Postdoctoral Scholar, 2020–2022.
- Michigan State University, Department of Chemistry, Research and Teaching Assistant, 2014–2020.
- Pontificia Universidad Católica del Perú, Faculty of Science and Engineering, Physics and Chemistry Teaching Assistant, 2013–2014.
- Linux Security S.A.C., IT Technician, 2009–2014.

Research experience

- June 2020 – June 2022, Postdoctoral Scholar, Division of Chemistry and Chemical Engineering, California Institute of Technology (Advisor Thomas F. Miller III). My research focused on the development and implementation of an inexpensive, semi-empirical method for computing the energies of periodic systems, based on the extended tight-binding method (GFN1-xTB) originally introduced by Prof. Stephan Grimme's group. This work was carried out in C++ within the Qcore software suite (Entos Inc.). I also refactored and streamlined the Python training tools for the Molecular-Orbital-Based Machine Learning (MOB-ML) method developed in Prof. Miller's group.
- January 2015 – May 2020, Ph.D. Student, Department of Chemistry, Michigan State University (Advisor Piotr Piecuch). I worked on the development of novel coupled-cluster (CC) and equation-of-motion coupled-cluster (EOMCC) approaches, which are among the most accurate methods in electronic structure theory. Specifically, I developed stochastically enhanced variants of CC and

EOMCC that exploit the leading components of the Full Configuration Interaction Quantum Monte Carlo (FCIQMC) wave function. This work was implemented in modern Fortran with bindings to C++ and Python.

- March 2012 – July 2014, Undergraduate Research Assistant, Department of Chemistry, Pontificia Universidad Católica del Perú (Advisor Eric Cosio). I worked on the characterization of epicuticular waxes found on the leaves of the myrmecophyte tree *Triplaris americana* using gas chromatography and mass spectrometry methods, as a contribution to the broader research field of plant-ant interactions from the chemical ecology perspective.
- October 2011 – January 2012, Undergraduate Visiting Research Assistant, Department of Chemistry, Eberhard Karls University of Tübingen (Advisor Thomas Chassé and Maria Benedetta Casu). I assisted Ph.D. students in characterizing substituted pentacene nanorods using X-ray photo-electron spectroscopy (XPS), ultraviolet photo-electron spectroscopy (UPS), low energy electron diffraction (LEED), and atomic force microscopy (AFM) under ultra-high vacuum conditions.
- July 2008 – July 2010, Voluntary Undergraduate Research Assistant, Department of Chemistry, Pontificia Universidad Católica del Perú (Advisor Javier Nakamatsu). I worked on refining inexpensive and efficient methods for depolymerizing PET and PC plastics, as part of a broader project on low-cost recycling techniques. During this period, I evaluated the use of household-grade microwave ovens to run depolymerization reactions and developed an Arduino-based device to improve the time logging of Ostwald viscometer measurements.

Awards and honors

- July 22–31, 2019, Invited instructor in the 2019 MolSSI Software Summer School, held at the Texas Advanced Computing Center (TACC), Austin, Texas.
- July 2019, 10th Congress of the International Society for Theoretical Chemical Physics in Tromsø Norway (ISTCP-X), Best Poster Award sponsored by the Journal of Computational Chemistry and the International Journal of Quantum Chemistry.
- January 2019 – June 2020, Molecular Sciences Software Institute Phase-II Software Fellow.
- July 2018 – December 2018, Molecular Sciences Software Institute Phase-I Software Fellow.
- June 2018, 50th Midwest Theoretical Chemistry Conference at the University of Chicago, Best Student Poster Award Sponsored by the Journal of Physical Chemistry.
- April 2018, College of Natural Science Continuation Fellowship for the Summer Semester of 2018.
- May 2016, Education Merit Award for Excellence in Teaching for the Spring Semester of 2016, Exceptional Award.

Grants and Contracts

- 2026, $230,000 subcontract from Michigan State University to Examol Corporation in support of the DARPA-sponsored NODES program.

Publications

1. A. Buccheri, R. Li, J.E. Deustua, S.M. Moosavi, P.J. Bygrave, and F.R. Manby, "Periodic GFN1-xTB Tight Binding: A Generalized Ewald Partitioning Scheme for the Klopman–Ohno Function" *J. Chem. Theory Comput.* **21**, 1615 – 1625 (2025).
https://doi.org/10.1021/acs.jctc.4c01234

2. L. Cheng, J. Sun, J.E. Deustua, V.C. Bhethanabotla, and T.F. Miller III, "Molecular-Orbital-Based Machine Learning for Open-Shell and Multi-Reference Systems with Kernel Addition Gaussian Process Regression" *J. Chem. Phys.* **157**, 154105 (2022).
https://doi.org/10.1063/5.0110886

3. 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).
https://doi.org/10.1063/5.0100165

4. F. Lu, L. Cheng, R. J DiRisio, J.M. Finney, M.A. Boyer, P. Moonkaen, J. Sun, S.J.R. Lee, J.E. Deustua, T.F. Miller III, A.B. McCoy, "Fast Near Ab Initio Potential Energy Surfaces Using Machine Learning" *J. Phys. Chem. A* **126**, 4013 (2022).
https://doi.org/10.1021/acs.jpca.2c02243

5. 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).
https://doi.org/10.1063/5.0064400

6. 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 – 4027 (2021).
https://doi.org/10.1021/acs.jctc.1c00181

7. J.E. Deustua, J. Shen, and P. Piecuch, "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions: Further Details and Comparisons" *J. Chem. Phys.* **154**, 124103-1 – 124103-25 (2021).
https://doi.org/10.1063/5.0045468

8. J.J. Eriksen et al., "The Ground State Electronic Energy of Benzene" *J. Phys. Chem. Lett.* **11**, 8922 – 8929 (2020).
https://doi.org/10.1021/acs.jpclett.0c02621

9. 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).
https://doi.org/10.1080/00268976.2020.1817592

10. G.M.J. Barca et al., "Recent Developments in the General Atomic and Molecular Electronic Structure System," *J. Chem. Phys.* **152**, 154102-1 – 154102-26 (2020).
https://doi.org/10.1063/5.0005188

11. J.E. Deustua, S.H. Yuwono, J. Shen, and P. Piecuch, "Communication: Accurate Excited-State Energetics by a Combination of Monte Carlo Sampling and Equation-of-Motion Coupled-Cluster Computations," *J. Chem. Phys.* **150**, 111101-1–111101-7 (2019).
https://doi.org/10.1063/1.5090346

12. J.E. Deustua, I. Magoulas, J. Shen, and P. Piecuch, "Communication: Approaching Exact Quantum Chemistry by Cluster Analysis of Full Configuration Quantum Monte Carlo Wave Functions," *J. Chem. Phys.* **149**, 151101-1–151101-6 (2018). https://doi.org/10.1063/1.5055769

13. J.E. Deustua, J. Shen, and P. Piecuch, "Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," *Phys. Rev. Lett.* **119**, 223003-1–223003-5 (2017). https://doi.org/10.1103/PhysRevLett.119.223003

Presentations given by J.E. Deustua

1. J.E. Deustua, I. Magoulas, S.H. Yuwono, J. Shen, and P. Piecuch, "Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster and Equation-of-Motion Coupled-Cluster Computations," 10th Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), Tromsø, Norway, July 11-17, 2019 [poster presentation].

2. J.E. Deustua, J. Shen, and P. Piecuch, "Cálculos de Energías Electrónicas de Alta Precisión Mediante Estimaciones Estocásticas de la Función de Onda y Computaciones Determinísticas de Coupled-Cluster," Chemistry Seminar, Pontificia Universidad Católica del Perú, Lima, Perú, May 23, 2019 [invited talk].

3. J.E. Deustua, J. Shen, and P. Piecuch, "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 50th Midwest Theoretical Chemistry Conference, University of Chicago, Chicago, Illinois, U.S.A., June 21-23, 2018 [poster presentation].

4. J.E. Deustua, J. Shen, and P. Piecuch, "Benchmarking Completely Renormalized Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies against Active-Space EOMCCSDt and Full EOMCCSDT Data," 49th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 1-3, 2017 [poster presentation].

5. J.E. Deustua, A.O. Ajala, J.A. Hansen, and P. Piecuch, "Benchmarking the Active-Space and Completely Renormalized Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies," International Society for Theoretical Chemical Physics Conference, Grand Forks, North Dakota, U.S.A., July 17-22, 2016 [poster presentation].

Presentations given by co-authors

1. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Tenth Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), symposium entitled "Emergent Electronic Structure Methods," Tromsø, Norway, July 11-17, 2019 [invited talk given by P. Piecuch].

2. P. Piecuch, J.E. Deustua, and J. Shen, "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," The symposium "Strong Correlation in Electronic Structure Theory," A Satellite Symposium to the 16th International Congress of Quantum Chemistry, Strasbourg, France, June 24-27, 2018 [invited talk given by P. Piecuch].

3. P. Piecuch, J.E. Deustua, and J. Shen, "Stochastic CC(P;Q) Theory: Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2017), Munich, Germany, August 27 - September 1, 2017 [invited talk given by P. Piecuch].

Software contributions

1. K. Gururangan, J.E. Deustua, and P. Piecuch. Research-level Python implementation of non-relativistic electronic structure calculations for molecular systems, based on ground-state coupled-cluster theory and its equation-of-motion extensions to excited, electron-attached, and ionized states. (https://github.com/piecuch-group/ccpy).
2. J.E. Deustua and others. Implementation of the periodic xTB method in the Qcore quantum chemistry software suite. Entos Inc., San Diego, CA. (https://entos.ai). Available since version 1.0.
3. J.E. Deustua. Python implementation of Wick's theorem, for the symbolic computation of expectation values of many-body operator products, using simple recursive rules. (https://github.com/edeustua/wickedtree).
4. J. Shen, J.E. Deustua, and P. Piecuch. Software implementation of the CC(t;3) approach in GAMESS (US) (https://www.msg.chem.iastate.edu/gamess/). Available since Public Release 2, August 2, 2018.
5. J.E. Deustua, J. Shen, and P. Piecuch. Software implementation of various CC methods with up to quadruply excited cluster components. (https://github.com/piecuch-group/ccq).
6. J.E. Deustua, J. Shen, and P. Piecuch. Software implementation of the CC(t;3) approach as an external plugin module for PSI4. (https://github.com/piecuch-group/cct3).
7. J.E. Deustua and K. Hunt. `pfedu`, an educational web tool that lets students visualize and analyze their homework results, built for Prof. Hunt's Molecular Thermodynamics course (CEM484) at Michigan State University. (https://github.com/edeustua/pfedu).

Technical experience

– Python, typescript, vuejs, AWS, Azure, GCP, Kubernetes | Examol Corporation
As the COO and founder engineer of Examol Corporation, I have written or co-written most of the foundational code. This spans the UI (vuejs), the backend in python (starlette), and the infrastructure (kubernetes with garden and timoni on GCP, AWS, and Azure), provisioned as IaaC via pulumi. I also manage the products and services associated with our startup. In addition to this engineering work, I have been running weighted ensemble (WE) and molecular dynamics (MD) simulations of membrane proteins, including G protein-coupled receptors (GPCRs).

– Python, typescript, vuejs, AWS | Emptor, Inc. - Emptor Dashboard
As a Software Engineer at Emptor, I was responsible for both the backend (python/flask) and the frontend (typescript with vuejs/nuxtjs) of the dashboard service, deployed on AWS via containers in ECS. My work included writing and deploying new features, as well as maintaining all the supporting systems, including the database, Redis, and message passing systems.

– C++, Python | Miller group - Qcore Entos
During my time in Prof. Miller's group, I implemented several algorithms and refactored code sections within the Qcore software suite (Entos Inc.), written in C++. This work made strong use of functional programming techniques to enforce immutability, consistent with Qcore's design philosophy of avoiding hard-to-debug side effects. Along the way, I debugged and improved many aspects of the CMake build scripts, contributing pull requests to open source projects such as `libecpint`.

– Python | Miller group - Qcore Entos
I set up a Python repository for training the Gaussian Process-based models that underpin the MOB-ML method. The package followed all standard Entos requirements: GitHub Actions CI, conda support, static analysis via `mypy`, and testing with `pytest`.

- Fortran, Python | Piecuch group - GAMESS(US)
  I have worked extensively in software development for research in the Piecuch group. Most of this work was implemented in modern Fortran and Python, within the Linux operating system, leveraging OpenMP, HDF5, and other HPC technologies.
- CUDA, MPI, HPC | High-Performance Computing Certificate
  As part of my High-Performance Computing Graduate Certificate at Michigan State University, I took courses in parallel computing with shared- and distributed-memory methods (OpenMP, MPI) as well as GPU programming (CUDA).
- Linux, IT | Piecuch group - MSU
  I also maintained and upgraded the computer systems available to the Piecuch group. This included acquiring, installing, and configuring new machines in the data center of the Chemistry Department at Michigan State University, namely a 96-core Skylake PowerEdge R940 and two 20-core Precision 7920 Dell systems.
- Linux, Windows, Mac, Networking
  As a technician at Linux Security S.A.C., I acquired a range of computer networking skills, including the implementation and configuration of firewalls (Endian, pfsense), network switches (basic VLANs), and routers, as well as troubleshooting network connectivity and security issues. I also troubleshot and maintained Windows, Mac, and Linux workstations.

Other information

Languages

- Spanish – Native language.
- English – Advanced. Certifications: Preliminary English Test (PET), First Certificate in English (FCE), and TOEFL.
- German – Intermediate. Certifications: German Kulturministerium Sprachdiplom Stufe 1 (A2/B1 level equivalent) and Stufe 2 (B2/C1 level equivalent).