Matthew R. Hennefarth

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Education

University of Chicago Sept 2021 — Present
Ph.D. Theoretical and Computational Chemistry
M.S. Chemistry

University of California, Los Angeles March 2020
B.S. Chemistry, Concentration in Physical Chemistry (Departmental Highest Honors)
B.S. Pure Mathematics
with College Honors and Latin Honors (*summa cum laude*)

Skills

- Expert in computational/quantum chemistry including catalysis, QM/MM, quantum dynamics, excited-state chemistry, CASSCF, DFT
- Developing open-source computational chemistry software in Python, C++, and Fortran (ex. PySCF, OpenMolcas)
- Experience with applying machine learning and active learning techniques to model chemical systems and reactivity
- Experience with developing and compiling software for and working on high-performance computing (HPC) clusters
- Experience with software development and tools (git/Github, make, cmake, UNIX)

Research Experience

Graduate Research Assistant July 2021 — Present
The University of Chicago, Department of Chemistry
Principle Investigator: Laura Gagliardi, lgagliardi@uchicago.edu

- Develop an efficient quantum electronic structure method (L-PDFT) including energy and analytical nuclear gradients in the open source softwares PySCF and OpenMolcas
- Implemented a PySCF interface to SHARC to study the nonradiative decay of molecular systems using nonadiabatic molecular dynamics using L-PDFT
- Develop a molecular dynamics technique combining high-level multireference methods and active learning neural networks for extended sampling of catalytic reactions

Staff Scientist April 2020 — June 2021
Undergraduate Research Scholar Sept 2018 — March 2020
University of California, Los Angeles, Department of Chemistry and Biochemistry
Principle Investigator: Anastassia N. Alexandrova, ana@chem.ucla.edu

- Built novel methodology and software in C++ (CPET) to quantify a protein's electric field topology to determine its impact on the catalytic rate and improve computationally designed enzymes
- Developed a mixed quantum mechanical/discrete molecular dynamics software (PHD3) to model metalloenzymes
- Utilize machine learning techniques to predict the catalytic rate of Diels-Alder enzymes trained on the reactant state electron density

Research Fellow May 2016 — Jan 2019
University of California, San Francisco, School of Dentistry
Principle Investigator: Sunita P. Ho, Sunita.Ho@ucsf.edu

- Perform elemental analysis using μXRF at the Advanced Light Source in Lawrence Berkeley National Laboratory to localize zinc-dependent inflammatory proteins to the mineralization-soft tissue interface
- Used X-ray, fluorescent, and electron microscopy techniques to create spatial-temporal maps of extracellular matrix and intracellular proteins tagged using immunohistochemistry

Publications

[1] **Hennefarth, M. R.**; Kim, Y.; Jangid, B.; Wardzala, J.; Hermes, M. R.; Truhlar, D. G.; Gagliardi, L. Hybrid Meta-GGA On-Top Functionals for Multiconfiguration Pair-Density Functional Theory Nuclear Gradients and Linearized Pair-Density Functional Theory Energies. **In Preparation**.

[2] Ajmera, P.; Vargas, S.; Chaturvedi, S. S.; **Hennefarth, M. R.**; Alexandrova, A. N. PyCPET – Computing Heterogeneous 3D Protein Electric Fields and Their Dynamics. *J. Chem. Theory Comput.* **Accepted**, DOI: 10.26434/chemrxiv-2024-r3thp.

[3] **Hennefarth, M. R.**; Truhlar, D. G.; Gagliardi, L. Semiclassical Nonadiabatic Molecular Dynamics of Azomethane using Linearized Pair-Density Functional Theory. *J. Chem. Theory Comput.* **2024**, DOI: 10.1021/acs.jctc.4c01061.

[4] **Hennefarth, M. R.**; Hermes, M. R.; Truhlar, D. G.; Gagliardi, L. Analytic Nuclear Gradients for Complete Active Space Linearized Pair-Density Functional Theory. *J. Chem. Theory Comput.* **2024**, DOI: 10.1021/acs.jctc.4c00095.

[5] **Hennefarth, M. R.**; King, D. S.; Gagliardi, L. Linearized Pair-Density Functional Theory for Vertical Excitation Energies. *J. Chem. Theory Comput.* **2023**, DOI: 10.1021/acs.jctc.3c00863.

[6] Manni, G. L. et al. The OpenMolcas Web: A Community-Driven Approach to Advancing Computational Chemistry. *J. Chem. Theory Comput.* **2023**, DOI: 10.1021/acs.jctc.3c00182.

[7] **Hennefarth, M. R.**; Hermes, M. R.; Truhlar, D. G.; Gagliardi, L. Linearized Pair-Density Functional Theory. *J. Chem. Theory Comput.* **2023**, DOI: 10.1021/acs.jctc.3c00207.

[8] Xian, W.; **Hennefarth, M. R.**; Lee, M. W.; Do, T.; Lee, E. Y.; Alexandrova, A. N.; Wong, G. C. Histidine-Mediated Ion Specific Effects Enable Salt Tolerance of a Pore-Forming Marine Antimicrobial Peptide. *Angew. Chem.* **2022**, DOI: 10.1002/anie.202108501.

[9] Ustriyana, P.; **Hennefarth, M. R.**; Srirangapatanam, S.; Jung, H.; Wany, Y.; Lue, T. F.; Kang, M.; Stoller, M. L.; Ho, S. P. Mineralized Peyronie's plaque has a phenotypic resemblance to bone. *Acta Biomater.* **2022**, DOI: 10.1016/j.actbio.2021.11.025, *The highlighted authors are joint first authors with equal contributions.*

[10] **Hennefarth, M.**; Alexandrova, A. Advances in Optimizing Enzyme Electrostatic Preorganization. *Curr. Opin. Struct. Biol.* **2022**, DOI: 10.1016/j.sbi.2021.06.006.

[11] Vargas, S.; **Hennefarth, M. R.**; Liu, Z.; Alexandrova, A. N. Machine Learning to Predict Diels–Alder Reaction Barriers from the Reactant State Electron Density. *J. Chem. Theory Comput.* **2021**, DOI: 10.1021/acs.jctc.1c00623.

[12] **Hennefarth, M. R.**; Alexandrova, A. N. Heterogeneous Intramolecular Electric Field as a Descriptor of Diels–Alder Reactivity. *J. Phys. Chem. A* **2021**, DOI: 10.1021/acs.jpca.1c00181.

[13] **Hennefarth, M. R.**; Alexandrova, A. N. Direct Look at the Electric Field in Ketosteroid Isomerase and Its Variants. *ACS Catal.* **2020**, DOI: 10.1021/acscatal.0c02795.

[14] Reilley, D. J.; **Hennefarth, M. R.**; Alexandrova, A. N. The Case for Enzymatic Competitive Metal Affinity Methods. *ACS Catal.* **2020**, DOI: 10.1021/acscatal.9b04831.

[15] **Hennefarth, M. R.**; Chen, L.; Wang, B.; Lue, T. F.; Stoller, M. L.; Lin, G.; Kang, M.; Ho, S. P. Physicochemical and biochemical spatiotemporal maps of a mouse penis. *J. Biomech.* **2020**, DOI: 10.1016/j.jbiomech.2020.109637.

[16] François-Moutal, L.; Jahanbakhsh, S.; Nelson, A. D.; Ray, D.; Scott, D. D.; **Hennefarth, M. R.**; Moutal, A.; Perez-Miller, S.; Ambrose, A. J.; Al-Shamari, A., et al. A chemical biology approach to model pontocerebellar hypoplasia type 1B (PCH1B). *ACS Chem. Biol.* **2018**, DOI: 10.1021/acschembio.8b00745.

Conference Poster and Oral Presentations

[1] **Hennefarth, M. R.**; King, D. S.; Hermes, M. R.; Truhlar D. G.; Gagliardi, L. "Linearized Pair-Density Functional Theory." 17th International Congress of Quantum Chemistry, **2023**.

[2] **Hennefarth, M. R.**; Hermes, M. R.; Truhlar D. G.; Gagliardi, L. "Linearized Pair-Density Functional Theory." 62nd Sanibel Symposium, **2023**.

[3] **Hennefarth, M. R.**; Vargas, S.; Liu, Z.; Fuller III, J. T.; Alexandrova, A. N. "Reactant State Electron Density Topology as a Descriptor of Chemical Reactivity." IUPAC Canadian Chemistry Conference and Exhibition, **2021**.

[4] **Hennefarth, M. R.**; Alexandrova, A. N. "Quantifying Perturbations in the Local Electric Field in Ketosteroid Isomerase." UCLA Undergraduate Research Showcase, **2020**.

[5] **Hennefarth, M. R.**; Chen, L.; Hsi, R.; Kang, M.; Reed-Maldonado, A.; Lin, G.; Stoller, M.; Lue, T.; Ho, S. "MP56-18 The Mouse Corpus Cavernosum Glandus is Biomechanically Analogous to the Human Corpus Cavernosum." Annual American Urology Association Conference, **2017**.

Awards and Honors

NSF Graduate Research Fellow, *National Science Foundation* Sept 2023 — Sept 2026
Olshansky Graduate Student Travel Award, *UChicago* June 2023
Eckhardt Scholar, *UChicago* Sept 2021 — Sept 2026
McCormick Fellow, *UChicago* Sept 2021
Dolores Cannon Southam Commencement Award for Excellence in Research, *UCLA* June 2020
UCLA Undergraduate Research Scholar, *UCLA* Sept 2019 — June 2020
Daniel Kivelson Research Fellow, *UCLA* June 2019 — Sept 2019
Dean Honor List, *UCLA* Dec 2016 — March 2020

Teaching

Co-Instructor, CHEM 368 Quantum Molecular and Materials Modeling, *UChicago* March 2024 — June 2024
Cross-listed course with CHEM 268, MENG 255, and MENG 355.
Teaching Assistant, CHEM 113: General Chemistry III, *UChicago* April 2022 — June 2022
Teaching Assistant, CHEM 112: General Chemistry II, *UChicago* Jan 2022 — March 2022
Teaching Assistant, CHEM 111: General Chemistry I, *UChicago* Sept 2021 — Dec 2021
Learning Assistant, CHEM 30B: Organic Chemistry II, *UCLA* June 2019 — Sept 2019
Learning Assistant, CHEM 14D: Organic Reactions and Pharmaceuticals, *UCLA* April 2019 — June 2019
Learning Assistant, CHEM 14C: Structure of Organic Molecules, *UCLA* Jan 2019 — March 2019
Learning Assistant, CHEM 30C: Organic Chemistry III, *UCLA* April 2018 — June 2018

Services

Reviewer for International Journals
ACS Omega, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Journal of Emerging Investigators
Senior Associate Editor, *Journal of Emerging Investigators* Aug 2022 — Present
Finance Director, *Los Angeles Student Education Outreach* Sept 2016 — March 2020
Mentor and tutor at-risk middle school students at Berendo Middle School in Los Angeles. Apply for funding to ensure proper funding for all of the organization's activities.