Matthew R. Hennefarth

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Education

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

University of Chicago Sept 2021 — Sept 2022
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

Computational Chemistry Programs: PySCF, OpenMolcas, SHARC, Turbomole, Gaussian, ORCA, and NAMD
Coding Languages: C++, Python, Fortran, UNIX Shell
Open Source Projects Contributed To: PySCF, OpenMolcas, Matplot++, phd3
Technical Skills: Electron microscopy (field emission and scanning transmission), energy dispersive X-ray spectroscopy, immunohistochemistry, light and fluorescent microscopy, and X-ray fluorescent spectroscopy

Research Experience

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

- Develop and implement an efficient linearized pair-density functional theory (L-PDFT) including energy and analytical nuclear gradients to study the photodynamics and photochemistry of systems with complex electronic structures
- Contributed and verified a PySCF interface to SHARC to enable nonadiabatic molecular dynamics with surface hopping or Ehrenfest dynamics using various L-PDFT
- Implemented *ab initio* Born-Oppenheimer molecular dynamics within PySCF for NVE- and NVT-ensembles
- Developed 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 (CPET) to quantify and probe a protein's locally produced electric field to determine its electrostatic preorganization
- Rewrote a distributable version of a mixed quantum mechanical/molecular dynamics software for proteins, phd3 (Protein Hybrid Discrete Dynamics/DFT), that includes a titratable feature
- Investigate the preferential binding of histidine and cations to phospholipid head groups over lysine to determine the mechanism by which anti-microbial proteins function using DFT
- Utilize the Quantum Theory of Atoms in Molecules to analyze critical points of the electron density within enzyme active sites and map differences to changes in the electrostatic preorganization

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

- Investigated possible cellular and mechanical mechanisms by which Peyronie's plaque is manifested using advanced correlative microscopy techniques
- Used 3D image analysis in Avizo, and light and fluorescent microscopy techniques to create spatial-temporal maps of extracellular matrix and intracellular proteins
- Performed elemental analysis and electron diffraction experiments at the Advanced Light Source in Lawrence Berkeley National Laboratory

Undergraduate Research Assistant Sept 2017 — June 2018

University of California, Los Angeles, Department of Chemistry and Biochemistry
Principle Investigator: Carla Koehler, koehler@chem.ucla.edu

- Assisted in various molecular biology techniques including zebrafish genotyping and plasmid sequencing to create protein KO lines
- Collaborated with the California Nanoscience Institute for high resolution fluorescent microscopy analysis of key proteins within the primary motor neuron mitochondria
- Established tools and software to quantify fluorescent images of various zebrafish KO lines

Publications

[1] Mitra, A.; Verma, S.; Otis, L.; Wang, Q.; Haldar, S.; **Hennefarth, M. R.**; D'Cunha, R.; Jangid, B.; Agarawal, V.; Hermes, M. R.; Gagliardi, L. Multireference Embedding on Classical and Quantum Computers. **In Preparation**.

[2] King, D. S.; **Hennefarth, M. R.**; Hermes, M. R.; Wardzala, J.; Sauza-de la Vega, A.; Agarawal, V.; Verma, S.; Gagliardi, L. Efficient Routes Through Configuration Space: Expanding the Capabilities and Applications of Multireference Methods. **In Preparation**.

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

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

[5] **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.

[6] **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.

[7] 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.

[8] **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.

[9] 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.

[10] 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.*

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

[12] 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.

[13] **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.

[14] **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.

[15] 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.

[16] **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.

[17] 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.