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*)

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 to study the photodynamics and photochemistry of systems with complex electronic structures
- Contributed to the development of compressed multistate pair-density functional theory non-adiabatic coupling vectors in *PySCF* and *OpenMolcas*
- Implemented *ab initio* Born-Oppenheimer molecular dynamics within *PySCF* for NVE-ensembles

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

- Develop new methods and software (*CPET*) to quantify and probe a protein's locally produced electric field to determine its electrostatic preorganization
- Rewrote a distributable version of our mixed quantum mechanical/molecular dynamics software for proteins, *phd3* (Protein Hybrid Discrete Dynamics/DFT), that includes a titratable feature
- Perform quantum mechanical calculations to investigate the preferential binding of histidine and cations to phospholipid head groups over lysine to determine the mechanism by which anti-microbial proteins function
- Utilize the Quantum Theory of Atoms in Molecules (QTAIM) to analyze critical points of the electron density within enzyme active sites and looking for differences which correspond 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

Publications

[1] **Hennefarth, M. R.**; Hermes, M. R.; Truhlar, D. G.; Gagliardi, L. Analytic Nuclear Gradients for Complete Active Space Linearized Pair-Density Functional Theory. **In Preparation**.

[2] **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.

[3] 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.

[4] **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.

[5] 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: doi.org/10.1002/anie.202108501.

[6] 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: doi.org/10.1016/j.actbio.2021.11.025, *The highlighted authors are joint first authors with equal contributions.*

[7] **Hennefarth, M.**; Alexandrova, A. Advances in Optimizing Enzyme Electrostatic Preorganization. *Curr. Opin. Struct. Biol.* **2022**, *72*, 1–8, DOI: 10.1016/j.sbi.2021.06.006.

[8] 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**, *17*, 6203–6213, DOI: 10.1021/acs.jctc.1c00623.

[9] **Hennefarth, M. R.**; Alexandrova, A. N. Heterogeneous Intramolecular Electric Field as a Descriptor of Diels–Alder Reactivity. *J. Phys. Chem. A* **2021**, *125*, 1289–1298, DOI: 10.1021/acs.jpca.1c00181.

[10] **Hennefarth, M. R.**; Alexandrova, A. N. Direct Look at the Electric Field in Ketosteroid Isomerase and Its Variants. *ACS Catal.* **2020**, *10*, 9915–9924, DOI: 10.1021/acscatal.0c02795.

[11] Reilley, D. J.; **Hennefarth, M. R.**; Alexandrova, A. N. The Case for Enzymatic Competitive Metal Affinity Methods. *ACS Catal.* **2020**, *10*, 2298–2307, DOI: 10.1021/acscatal.9b04831.

[12] **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**, *101*, 109637, DOI: 10.1016/j.jbiomech.2020.109637.

[13] 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**, *13*, 3000–3010, DOI: 10.1021/acschembio.8b00745.

Conference Poster and Oral Presentations

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

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

[5] **Hennefarth, M. R.** (Presenter); 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**.

[6] **Hennefarth, M. R.**; Chen, L.; Kang, M.; Hsi, R.; Reed-Maldonado, A.; Lin, G.; Stoller, M.; Lue, T.; Ho, S. (Presenter) "PD31-11 The Origins of Calcified Peyronie's Plaque." 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, *The University of Chicago* June 2023
Eckhardt Scholar, *The University of Chicago* Sept 2021 — Sept 2026
McCormick Fellow, *The University of Chicago* 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 and Services

Reviewer for International Journals
Journal of Physical Chemistry, Journal of Chemical Theory and Computation, Journal of Emerging Investigators
Senior Associate Editor, *Journal of Emerging Investigators* Aug 2022 — Present
Comprehensive General Chemistry Teaching Assistant, *The University of Chicago* Sept 2021 — June 2022
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.
Organic Chemistry Learning Assistant, *UCLA* April 2018 — Aug 2019
Facilitated student learning by encouraging active dialogue in problem solving in organic chemistry. Create practice problems for discussion sections as well as create and lead the final review session.

Skills

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