Laura M. Weiler

Graduate Student, Departments of Chemistry, Stanford University
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EDUCATION

Ph.D. Chemistry **September 2022 – present**
Stanford University, Stanford, CA

Bachelor of Science in Physics & **August 2018 – May 2022**
Bachelor of Arts in Computer Science **GPA: 3.74 (4.0 scale)**
University of Iowa, Iowa City, IA

RESEARCH EXPERIENCE

Graduate Research Assistant **August 2022 – present**
Department of Chemistry, Stanford University, Stanford, CA
Advisor: Prof. Todd Martínez

Undergraduate Research Assistant **May 2019 – July 2022**
Department of Chemistry, University of Iowa, Iowa City, IA
Project: Exploring machine learning for interactions in metals
Advisor: Prof. James Shepherd

Undergraduate Research Assistant **January – May 2020**
Department of Computer Science, University of Iowa, Iowa City, IA
Project: Exploring greedy and parallel variants of bio-inspired optimization algorithms
Advisor: Prof. Suely Oliveira

RESEARCH INTERESTS

The past decade's advances in computer hardware and software have facilitated vertical growth in computer simulation techniques for chemical systems. The goal of the next decade should be to similarly facilitate horizontal growth- seamlessly connecting simulation techniques for chemical systems at different time and length scales in order to accurately and affordably model real-world systems. I seek to leverage my education and research experience to help make full-scale chemical modeling routine to the benefit of drug discovery and materials design.

AWARDS AND FELLOWSHIP

Stanford Graduate Fellow (2022-2026) **March 2022**
Department of Physics and Astronomy James A. Van Allen Award **November 2021**
ACS Division of Physical Chemistry Award **May 2021**
Iowa Center for Research by Undergraduates Research Fellow (2021-2022) **March 2021**
Vice President for Research Excellence in Undergraduate Research Award **March 2021**
Best Poster Award APS Prairie Section Meeting **November 2020**
Iowa Center for Research by Undergraduates Research Fellow (2020-2021) **August 2020**

PUBLICATIONS

6. Van Benschoten, W. Z., **Weiler, L.**, Smith, G. J., Man, S., DeMello, T., Shepherd, J. J. (2022). Electronic specific heat capacities and entropies from density matrix quantum Monte Carlo using Gaussian process regression to find gradients of noisy data. Submitted.

5. Mihm, T. N., **Weiler, L.**, Shepherd, J. J. (2022). How the exchange energy can affect the power laws used to extrapolate the coupled cluster correlation energy to the thermodynamic limit. Submitted.

4. **Weiler, L.**, Mihm, T. N., Shepherd, J. J. (2022). Machine learning for a finite size correction in periodic coupled cluster theory calculations. The Journal of Chemical Physics, 156, 204109; https://doi.org/10.1063/5.0086580

3. Mihm, T. N., Schäfer, T., Ramadugu, S. K., **Weiler, L.**, Grüneis, A., Shepherd, J. J. (2021). A shortcut to the thermodynamic limit for quantum many-body calculations of metals. Nature Computational Science 1, 801–808; https://doi.org/10.1038/s43588-021-00165-1

PUBLICATIONS (conference papers)

2. *Hajewski, J., *Oliveira, S., *Stewart, D. E., & ***Weiler, L.** (2021). Exploring Trade-offs in Parallel Beam-ACO. 2021 IEEE 11th Annual Computing and Communication Workshop and Conference. IEEE, pp. 1525. https://doi.org/10.1109/CCWC51732.2021.9376177 * authors listed alphabetically

1. *Hajewski, J., *Oliveira, S., *Stewart, D. E., & ***Weiler, L.** (2020). GBeam-ACO: a greedy and faster variant of Beam-ACO. Proceedings of the 2020 Genetic and Evolutionary Computation Conference Companion. ACM, pp. 434. https://doi.org/10.1145/3377929.3398081 * authors listed alphabetically

PRESENTATIONS (national)

5. **Weiler, L**. Mihm, T., Shepherd, J. J. *Machine learning for correcting finite-size errors in coupled cluster correlation energies*, presented virtually at the American Chemical Society Fall meeting 2021

4. **Weiler, L.**, Mihm, T., Shepherd, J. J. Applying Neural Networks and Gaussian Process Regression to the Transition Structure Factor, presented virtually at the American Physical Society March Meeting 2021

3. **Weiler, L.,** Mihm, T., Shepherd, J. J. *Using Gaussian Process Regression to Integrate the Transition Structure Factor Curve for the Many-Body Correlation Energy*, presented at the American Physical Society Prairie Section Meeting 2020, hosted by Illinois Institute of Technology, Chicago, IL

2. **Weiler, L.**, Mihm, T., Shepherd, J. J. *Machine learning algorithms for the coupled cluster correlation energy in the uniform electron gas*, presented at the Virtual Conference on Theoretical Chemistry (VCTC) 2020, hosted by Stanford University, Stanford, CA

1. **Weiler, L.**, Mihm, T., Shepherd, J. J. *Frozen core coupled cluster calculations on finite electron gases*, presented at the Virtual Electronic Structure Workshop (ESW) 2020, hosted by University of California-Merced, Merced, CA