E. Adrian Henle, Ph.D.

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Work Experience

- **Oregon State University** *2019 – 2024* Graduate Teaching/Research Assistant
  Scientific application development and documentation in interdisciplinary collaborations between chemistry, chemical engineering, and computer science. Julia, PyTorch, MATLAB, COMSOL, GitHub CI, developer relations, graph neural networks, LLMs. Classroom, laboratory, and online course development and instruction; direct mentorship of undergraduate and junior graduate researchers.
- **University of Washington** *2017 – 2020* Extension Lecturer, Professional and Continuing Education
  Online student instruction and curriculum development in data science and machine learning.
- **Nanovox, LLC** *2017 – 2019* Staff Scientist
  Nanotechnology R&D and 3D printing of nanomaterial composites. Built and operated chemical reactors. Developed software and hardware for process control, safety, and data analysis. Electron microscopy, X-ray spectroscopy/diffractometry, Quantum ESPRESSO, Python, Arduino, LabVIEW, and IoT.
- **University of Oregon** *2012 – 2015* Graduate Teaching Fellow
  Advanced organic, inorganic, and organometallic synthesis, mass spectrometry, and computational chemistry (DFT and MD using Spartan, Gaussian, and LAMMPS). Instructed undergraduate and graduate students in classroom and laboratory settings. Supervised undergraduate and graduate researchers.
- **Seattle University** *2011 – 2012* Undergraduate Research Assistant
  Organometallic synthesis, air-free handling, photochemistry, electrochemistry, and spectroscopy.
- **Lawrence Berkeley National Laboratory** *2005 – 2008* Lab Assistant
  Biology, biochemistry, sterile handling, and visible, fluorescence, and X-ray microscopy.

Education

- **Ph.D. Chemical Engineering** *2024* Oregon State University
- **B.S. Computer Science** *2017* Oregon State University
- **M.S. Chemistry** *2015* University of Oregon
- **B.S. Chemistry** *2012* Seattle University

Publications & Patents

- **SomMOLier.jl: Leveraging Natural Language Information for Zero-Shot Odorant Classification**
  E. A. Henle, X. Z. Fern, C. M. Simon
  2024 (manuscript in preparation)
- **Tuning Enantioselective Drug Adsorption in Isoreticular Homochiral Metal-Peptide Frameworks through Proximity Pore Interactions**
  J. Ho, A. Yadav, A. Gladysiak, A. Carpenter, A. Verma, A. Henle, M. Subramanian, J. Baio, K. Stylianou
  Chem. Mater. 2024 (submitted)
  DOI: 10.26434/chemrxiv-2023-9b9hj
- **Selective Xenon Recovery Using Aluminum-Based MOFs with Conserved Pore Topology**
  T. Hurley, A. Henle, A. Gladysiak, V. T. Remcho, K. C. Stylianou
  ACS Appl. Mater. 2024 (accepted)
  DOI: 10.1021/acsami.4c06215

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Publications & Patents (continued)

- **Methods and Apparatus for Synthesis and Magnetophoretic Fractionization Size-Selection of Magnetic Nanoparticles from a Solution**
  P. G. Hugger, C. N. Teters, T. L. Allen, E. A. Henle, P. J. Polesnak
  US Patent 20,220,135,423 2022

- **Methods of Manufacturing Nanocomposite RF Lens and Radome**
  P. G. Hugger, C. N. Teters, E. A. Henle, T. L. Allen, J. P. Harmon, S. P. Grimm, E. W. Elliott, P. J. Polesnak
  US Patent 11,469,514 2022

- **Classifying the toxicity of pesticides to honey bees via support vector machines with random walk graph kernels**
  P. Yang, E. A. Henle, X. Z. Fern, C. M. Simon
  J. Chem. Phys. 2022 **157** (3), 034102
  DOI: 10.1063/5.0090573

- **Surviving the bridge in Squid Game**
  E. A. Henle, N. Gantzler, F. X. Coudert, C. Simon
  Chalkdust 2022 **15**

- **Non-equilibrium molecular geometries in graph neural networks**
  A. Raza, E. A. Henle, X. Fern
  ELLIS Machine Learning for Molecule Discovery 2022
  DOI: 10.48550/arXiv.2203.04697

- **PoreMatMod.jl: Julia Package for *in Silico* Postsynthetic Modification of Crystal Structure Models**
  E. A. Henle, N. Gantzler, P. K. Thallapally, X. Z. Fern, C. M. Simon
  J. Chem. Inf. Model. 2022 **62** (3), 423-432
  DOI: 10.1021/acs.jcim.1c01219

- **Non-injective gas sensor arrays: identifying undetectable composition changes**
  E. A. Henle, N. Gantzler, P. K. Thallapally, X. Z. Fern, C. M. Simon
  J. Phys.: Condens. Matter 2021 **33**, 464003
  DOI: 10.1088/1361-648X/ac1e49

- **Synthesis of Tetraphosphine Macrocycles Using Copper(I) Templates**
  B. P. Nell, C. D. Swor, E. A. Henle, L. N. Zakharov, N. I. Rinehart, A. Nathan, D. R. Tyler
  Dalton Transactions 2016 **45**, 8253-8264
  DOI: 10.1039/C6DT00758A

- **Selection for a Single Self-Assembled Macrocycle from a Hybrid Metal–Ligand Hydrogen-Bonded Ligand Subunit**
  S. K. Sommer, E. A. Henle, L. N. Zakharov, M. D. Pluth
  Inorganic Chemistry 2015 **54** (14), 6910-6916
  DOI: 10.1021/acs.inorgchem.5b00857

- **Synthesis and Structures of Triple-Decker Complexes with a Bridging Tetramethylcyclopentadienyl Ligand**
  S. K. Ghag, M. L. Tarlton, E. A. Henle, E. M. Ochoa, A. W. Watson, L. N. Zakharov, E. J. Watson
  Organometallics 2013 **32** (6), 1851-1857
  DOI: 10.1021/om301258s