Daniel Tabor

Texas A&M University
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Professional Experience

2026- Associate Professor, Department of Chemistry, Texas A&M University

2019-2026 Assistant Professor, Department of Chemistry, Texas A&M University

2016-2019 Postdoctoral Fellow, Harvard University, Aspuru-Guzik Group

Education

2016 Ph.D. Chemistry, University of Wisconsin–Madison

Advisor: Edwin L. Sibert III

Thesis: Extracting Structural Information from the OH and CH Stretch Spectral Regions with a Local Mode Approach

2011 B.S. Chemistry University of Texas at Austin

Advisor: John F. Stanton

Undergraduate Thesis: High-Accuracy Extrapolated Ab Initio Thermochemistry of Closed and Open Shell Molecules

Publications

*Independent Career, Corresponding Authors Indicated with **

Current Preprints/In Press Articles

27. A.F. Moody, V.S. Jeyaraj, **D.P. Tabor**,* Predicting Amide-I Infrared Spectra Directly from Coarse-Grained Protein Simulations, ChemRXiv Preprint. DOI: https://chemrxiv.org/doi/full/10.26434/chemrxiv.15005613/v1 (2026).

26. A. Khambhawala, S. Rekhi, Q. Chen, P. Mohanty, **D.P. Tabor**, J. Mittal,* Learning molecular determinants of selective small-molecule partitioning across biomolecular condensates, bioRxiv Preprint 2026.05.23.727301 DOI: https://doi.org/10.64898/2026.05.23.727301 (2026).

Published in Peer-Reviewed Journal

25. C. Lee, E. Brenneman, K. Au, A.P. Baldo, J.M. Rimsza, M.A. Boyer, K. Bowman-James, **D.P. Tabor**,* T.S. Zwier,* Adaptive Halide Binding with Anion Size: Triggering Chiral D3 to Trigonal Prism Changes in a Molecular Cage, *J. Am. Chem. Soc.* **148**, 34938–34948 (2026). DOI: https://doi.org/10.1021/jacs.6c11035

24. M. Avais, C. Wang, R.M. Thakur, K.G. Schoonover, V.S. Jeyaraj, **D.P. Tabor**, J.L. Lutkenhaus,* and E.B. Pentzer,* Tacticity-Regulated Electrochemical Properties of Poly(2,2,6,6-tetramethylpiperidinyloxy Methacrylate), *J. Am. Chem. Soc.* **148**, 22621–22629 (2026). DOI: https://doi.org/10.1021/jacs.6c01504

23. M.A. Boyer* and **D.P. Tabor**,* Construction of Arbitrary Order Internal Coordinate Transformations to Improve Studies of Large Amplitude Motions, J. Phys. Chem. A 130, 36803694 (2026).
DOI: https://doi.org/10.1021/acs.jpca.6c00573 ChemRXiv Preprint DOI: 10.26434/chemrxiv-2026-bzmpw (2026).

22. H.A. Moran, A.F. Moody, M.A. Boyer, P. Garrett, M. Quiroz, S. Sanfui, M.Y. Darensbourg,* C.R. Baiz,* **D.P. Tabor**,* Low-cost Calculation and Analysis of 2D IR Spectra of Model Diiron Trinitrosyl Complexes in the NO Stretch Region with Vibrational Perturbation Theory, *Phys. Chem. Chem. Phys.* **28**, 5253-5264 (2026). DOI: 10.1039/D5CP03578C. ChemRXiv Preprint DOI: 10.26434/chemrxiv-2025-nmjrl (2025).

21. C.B. Somodi, V. Satheesh, T.-H. Chao, **D.P. Tabor**, E.B. Pentzer,* P.S. Shamberger,* Selective Deuteration of Neopentyl Glycol and its Effect on the Plastic Crystal Transformation, *J. Phys. Chem. B* **130**, 20052014 (2026). DOI: 10.1021/acs.jpcb.5c08152. ChemRXiv Preprint DOI: 10.26434/chemrxiv-2025-w5vfl (2025).

20. J.S.-J. Yang, V.S. Jeyaraj, G. Ma, D.D. Doria, X. Gu,* **D.P. Tabor**,* L. Fang,* Synthesis and Persistence Length Study of Defect-Free and Non-Aggregated Conjugated Ladder Polymers, *JACS Au* **5**, 6210–6219 (2025). ChemRXiv Preprint DOI: 10.26434/chemrxiv-2025-3blt6 (2025).

19. T.-H. Chao, A. Foncerrada, P.J. Shamberger,* **D.P. Tabor**,* Low-Data Machine Learning Models for Predicting Thermodynamic Properties of Solid-Solid Phase Transformations in Plastic Crystals, *Soft Matter* **21**, 5957-5968 (2025).
DOI: https://doi.org/10.1039/D5SM00353A ChemRXiv Preprint: DOI: 10.26434/chemrxiv-2025-qk02t (2025).

18. C.-H. Li,* M. C. Kaymak, M. Kulichenko, N. Lubbers, B. Nebgen, S. Tretiak, J. Finkelstein, **D.P. Tabor**,* A. Niklasson,* Shadow Molecular Dynamics with a Machine Learned Flexible Charge Potential, *J. Chem. Theor. Comput.* **21** 3658-3675 (2025). DOI: https://doi.org/10.1021/acs.jctc.5c00062. ChemRXiv Preprint: DOI: 10.26434/chemrxiv-2025-x8b23 (2025).

17. N.P.D. Sawaya,* D. Marti-Dafcik, Y. Ho, **D.P. Tabor**, D. Bernal, A.B. Magann, S. Premaratne, P. Dubey, A. Matsuura, N. Bishop, W.A. de Jong, S. Benjamin, O.D. Parekh, N. Tubman, K. Klymko,* and D. Camps,* HamLib: A library of Hamiltonians for benchmarking quantum algorithms and hardware, *Quantum* **8**, 1559 (2024). DOI: https://doi.org/10.22331/q-2024-12-11-1559. arXiv preprint: arXiv:2306.13126 (2023).

16. A.D. Easley, C.-H. Li, S.-G. Li, T.P. Nguyen, K.-H. M. Kuo, K.L. Wooley,* **D.P. Tabor**,* and J.L. Lutkenhaus,* Electron Transport Kinetics for Viologen-containing Polypeptides with Varying Side Group Linker Spacing, *J. Mater. Chem. A*, **12**, 31871-31882 (2024). DOI: https://doi.org/10.1039/D4TA06766E

15. R. Alessandri, C.-H. Li, S. Keating, K.T. Mohanty, A. Peng, J.L. Lutkenhaus, S. J. Rowan, **D.P. Tabor**,* and J.J. de Pablo,* Structural, Ionic, and Electronic Properties of Solid-State Phthalimide-Containing Polymers for All-Organic Batteries, *JACS Au* **4**, 23002311 (2024). DOI: https://doi.org/10.1021/jacsau.4c00276 ChemRxiv Preprint: 10.26434/chemrxiv-2024-qkjr8 (2024).

14. C.B. Somodi, K. McCormick, **D.P. Tabor**, E.B. Pentzer, P.J. Shamberger,* Kinetics of the Plastic Crystal Transition in Neopentyl Glycol, *J. Appl. Phys.* **135**, 145101 (2024). DOI: https://doi.org/10.1063/5.0192791

13. R.W. Neisser, J.P. Davis, M.E. Alfieri, H. Harkins, A.S. Petit,* **D.P. Tabor**,* and N.M. Kidwell,* Photophysical Outcomes of Water-Solvated Heterocycles: Single-Conformation Ultraviolet and Infrared Spectroscopy of Microsolvated 2-Phenylpyrrole, *J. Phys. Chem. A* **127** (50), 10540–10554 (2023).
DOI: https://doi.org/10.1021/acs.jpca.3c04472

12. T. Ma, E. Fox, M. Ai, C.-H. Li, K.A.N. Sachinthani, K. Mohanty, **D.P. Tabor***, E.B. Pentzer,* and J.L Lutkenhaus,* Charge Transfer in Spatially Defined Organic Radical Polymers, *Chem. Mater.* **35**, 21, 9346-9351(2023).
DOI: https://doi.org/10.1021/acs.chemmater.3c02148

11. C.-H. Li and **D.P. Tabor**,* Generative Organic Electronic Molecular Design Informed by Quantum Chemistry. *Chem. Sci.* **14**, 11045-11055 (2023). DOI: 10.1039/D3SC03781A
ChemRxiv Preprint (2023). DOI: 10.26434/chemrxiv-2023-bgcjg-v2

10. T.-H. Chao, S. Rekhi, J. Mittal, and **D.P. Tabor**,* Data-Driven Models for Predicting Intrinsically Disordered Protein Polymer Physics Directly from Composition or Sequence. *Mol. Syst. Des. Eng.* **8**, 1146-1155 (2023).
DOI: https://doi.org/10.1039/D3ME00053B. ChemRxiv Preprint: 10.26434/chemrxiv-2023-wrnq1 (2023).

9. J. Li, B.-J. Peng, S. Li, **D.P. Tabor**, L. Fang,* and C.M. Schroeder,* Ladder-type conjugated molecules as robust multi-state single-molecule switches, *Chem*, **9**, 2282-2297 (2023). DOI: https://doi.org/10.1016/j.chempr.2023.05.001

8. T. Ma, C.-H. Li, R.M. Thakur, **D.P. Tabor**, and J.L. Lutkenhaus,* The role of the Electrolyte in Non-conjugated Radical Polymers for Metal-free Aqueous Energy Storage Electrodes, *Nat. Mater.* **22**, 495-502 (2023).
DOI: https://doi.org/10.1038/s41563-023-01518-z

7. C.-H. Li and **D.P. Tabor**,* Reorganization Energy Predictions with Graph Neural Networks Informed by Low-Cost Conformers, *J. Phys. Chem. A*, **127**, 3484–3489 (2023). DOI: https://doi.org/10.1021/acs.jpca.2c09030 ChemRxiv preprint at: 10.26434/chemrxiv-2022-fk22p

6. N.J. Shuber, **D.P. Tabor**, S.W. North,* Theoretical Investigation of the Ground State Dissociation Pathways of CH_2NO_2, *Chem. Phys.* **568** 111823 (2023).
DOI: https://www.sciencedirect.com/science/article/abs/pii/S0301010423000058

5. J. Lee, S. Li, X. Ji, S. Che, Y. Cao, **D.P. Tabor**,* L. Fang,* Molecular mechanism of rigidity- and planarity-promoted, state-dependent doping of conjugated ladder-type molecules, *Mater. Chem. Front.* **6**, 3329-3337 (2022). DOI: https://doi.org/10.1039/D2QM00789D

4. B. Peterson, M. Alfieri, D. Hood, C. Hettwer, D. Constantino, **D.P. Tabor**,* N.M. Kidwell,* Solvent-Mediated Charge Transfer Dynamics of a Model Brown Carbon Aerosol Chromophore: Photophysics of 1-Phenylpyrrole Induced by Water Solvation, *J. Phys. Chem. A* **126**, 4313–4325 (2022). ChemRxiv Preprint: 10.26434/chemrxiv-2022-4rt78.

3. G. Ma, M. Leng, S. Li, Z. Cao, Y. Cao, **D.P. Tabor**,* L. Fang,* and X. Gu,* Robust Chain Aggregation of Low-Entropy Rigid Ladder Polymer in Solution, *J. Mater. Chem. C* **10**, 13896-13904 (2022).
DOI: https://doi.org/10.1039/D2TC00761D

2. C.-H. Li and **D.P. Tabor**,* Discovery of lead low-potential radical candidates for organic radical polymer batteries with machine-learning-assisted virtual screening, *J. Mater. Chem. A* **10**, 8273-8282 (2022).
DOI: https://doi.org/10.1039/D2TA00743F. ChemRxiv Preprint: 10.26434/chemrxiv-2022-hlw2f.

1. N.P.D. Sawaya,* F. Paesani, and **D.P. Tabor**,* Near- and Long-Term Quantum Algorithmic Approaches for Vibrational Spectroscopy, *Phys. Rev. A* **104**, 062419 (2021). DOI: https://doi.org/10.1103/PhysRevA.104.062419
Preprint available at: arXiv:2009.05066

Work Prior to Independent Career

26. Q. Wang, Z. Yao, C. Zhao, T. Verhallen, **D.P. Tabor**, M. Liu, F. Ooms, F. Kang, A. Aspuru-Guzik, Y.-S. Hu, M. Wagemaker, and B. Li, Interface Chemistry of an Amide Electrolyte for Highly Reversible Lithium Metal Batteries, *Nat. Commun.* **11**, 4188 (2020). DOI: https://doi.org/10.1038/s41467-020-17976-x

25. C.F. Perkinson, **D.P. Tabor**, M. Einzinger, D. Sheberla, H. Utzat, T.-A. Lin, D.N. Congreve, M. Bawendi, A. Aspuru-Guzik, and M.A. Baldo, Discovery of Blue Singlet Exciton Fission Molecules via a High-Throughput Virtual Screening and Experimental Approach, *J. Chem. Phys.* **151**, 121102 (2019). DOI: https://doi.org/10.1063/1.5114789

24. **D.P. Tabor**, V. Chiykowski, P. Friederich, Y. Cao, D.J. Dvorak, C.P. Berlinguette, and A. Aspuru-Guzik, Design Rules for High Mobility Xanthene-Based Hole Transport Materials, *Chem. Sci.* **10**, 8360-8366 (2019). DOI: 10.1039/C9SC01491H

23. L. Tong, M.-A. Goulet, **D.P. Tabor**, E.F. Kerr, D. De Porcellinis, E.M. Fell, A. Aspuru-Guzik, R.G. Gordon, and M.J. Aziz, Molecular Engineering of an Alkaline Naphthoquinone Flow Battery, *ACS Energy Lett.* **4**, 1880-1887 (2019). DOI: https://doi.org/10.1021/acsenergylett.9b01321
Preprint: ChemRxiv doi:10.26434/chemrxiv.7732472.v1

22. **D.P. Tabor**†, R. Gómez-Bombarelli†, L. Tong, R.G. Gordon, M.J. Aziz, and A. Aspuru-Guzik, Mapping the Frontiers of Quinone Stability in Aqueous Media: Implications for Organic Aqueous Redox Flow Batteries, *J. Mater. Chem. A* **7**, 12833-12841 (2019). DOI: 10.1039/C9TA03219C.
Preprint: ChemRxiv doi:10.26434/chemrxiv.6990053.v2. †equal contribution.

21. M.-A. Goulet, L. Tong, D. A. Pollack, **D.P. Tabor**, S.A. Odom, A. Aspuru-Guzik, E.E. Kwan, R.G. Gordon and M.J. Aziz, Extending the Lifetime of Organic Flow Batteries via Redox State Management, *J. Am. Chem. Soc.* **141**, 8014-8019 (2019). DOI: 10.1021/jacs.8b13295

20. K. Alberi, M. Buongiorno Nardelli, A. Zakutayev, L. Mitas, S. Curtarolo, A. Jain, M. Fornari, N. Marzari, I. Takeuchi, M. Green, M. Kanatzidis, M. Toney, S. Butenko, B. Meredig, S. Lany, U. Kattner, A. Davydov, E. Toberer, V. Stevanovic, A. Walsh, N.G. Park, A. Aspuru-Guzik, **D.P. Tabor**, J. Nelson, J. Murphy, A. Setlur, J. Gregoire, H. Li, R. Xiao, A. Ludwig, L. Martin, A. Rappe, S.-H. Wei, and J. Perkins, The 2019 Materials by Design Roadmap, *J. Phys. D: Appl. Phys.* **52**, 013001 (2019). DOI: https://doi.org/10.1088/1361-6463/aad926

19. V. Chiykowski, Y. Cao, H. Tan, **D.P. Tabor**, E.H. Sargent, A. Aspuru-Guzik, and C.P. Berlinguette, Precise Control of Thermal and Redox Properties of Organic Hole-Transport Materials, *Angew. Chem. Int. Ed.* **57**, 15529 (2018). DOI: 10.1002/anie.201810809

18. D. Kwabi, K. Lin, Y. Ji, E.F. Kerr, M.-A. Goulet, D. De Porcellinis, **D.P. Tabor**, D.A. Pollack, A. Aspuru-Guzik, R.G. Gordon, and M.J. Aziz, Alkaline Quinone Flow Battery with Long Lifetime at pH 12, *Joule* **2**, 1894-1906 (2018). DOI: 10.1016/j.joule.2018.07.005 (Featured Article).

17. N.P.D. Sawaya, D. Rappoport, **D.P. Tabor**, and A. Aspuru-Guzik, Excitonics: A Set of Gates for Molecular Exciton Processing and Signaling, *ACS Nano* **12**, 6410-6420 (2018). DOI: 10.1021/acsnano.8b00584
Preprint: https://doi.org/10.26434/chemrxiv.5309617.v1

16. **D.P. Tabor**, Flow Batteries: Approaching Saturation Limits, *Nat. Energy*, **3**, 455-456 (2018). DOI: 10.1038/s41560-018-0169-1 (News and Views).

15. **D.P. Tabor**, L.M. Roch, S.K. Saikin, C. Kreisbeck, D. Sherberla, J.H. Montoya, S. Dwaraknath, M. Aykol, C. Ortiz, H. Tribukait, C. Amador-Bedolla, C.J. Brabec, B. Maruyama, K.A. Persson, and A. Aspuru-Guzik, Accelerating Discovery of Materials for Clean Energy in the Era of Smart Automation, *Nat. Rev. Mater.* **3**, 5-20 (2018). DOI: 10.1038/s41578-018-0005-z

14. Z. Yang, L. Tong, **D.P. Tabor**, E.S. Beh, M.-A. Goulet, D. De Porcellinis, A. Aspuru-Guzik, R.G. Gordon, and M.J. Aziz, Alkaline Benzoquinone Aqueous Flow Battery for Large-Scale Storage of Electrical Energy, *Adv. Energy Mater.* **8** 1702056 (2018). DOI: 10.1002/aenm.201702056

13. D.M. Hewett, **D.P. Tabor**, J.L. Fischer, E.L. Sibert III, and T.S. Zwier, IR-induced Fluorescence-Gain Spectroscopy: Conformation-Specific Excited State Infrared Spectra of the Alkylbenzenes, *J. Phys. Chem. Lett.* **8**, 5296-5300 (2017). DOI: 10.1021/acs.jpclett.7b02276

12. D.M. Hewett, S. Bocklitz, **D.P. Tabor**, E.L. Sibert III, M. Suhm, and T.S. Zwier, Identifying the First Folded Alkylbenzene: Ultraviolet, Infrared, and Raman Spectroscopy of Pentylbenzene through Decylbenzene, *Chem. Sci.* **8**, 5305 (2017). DOI: 10.1039/C7SC02027A

11. D.J. Bakker, A. Dey, **D.P. Tabor**, Q. Ong, J. Mahé, M.-P. Gaigeot, E.L. Sibert III, and A.M. Rijs, Fingerprints of Inter- and Intramolecular Hydrogen Bonding in Saligenin-Water Clusters Uncovered by Mid- and Far-Infrared Spectroscopy, *Phys. Chem. Chem. Phys.* **19**, 20343-20356 (2017). DOI: 10.1039/C7CP01951C

10. P.R. Franke, **D.P. Tabor**, C.P. Moradi, G.E. Douberly, J. Agarwal, H.F. Schaefer III, and E.L. Sibert III, Infrared Laser Spectroscopy of the *n*-Propyl and *i*-Propyl Radicals: Stretch-Bend Fermi Coupling in the Alkyl CH Stretch Region, *J. Chem. Phys.* **145**, 224304 (2016). DOI: 10.1063/1.4971239

9. J.A. Korn, **D.P. Tabor**, E.L. Sibert III, and T.S. Zwier, Conformation-Specific Spectroscopy of Alkyl Benzyl Radicals: Effects of a Radical Center on the CH Stretch Infrared Spectrum of an Alkyl Chain, *J. Chem. Phys.* **145**, 124314 (2016). DOI: 10.1063/1.4963227

8. **D.P. Tabor**, D.M. Hewett, S. Bocklitz, J.A. Korn, A.J. Tomaine, A.K. Ghosh, T.S. Zwier and E.L. Sibert III, Anharmonic Modeling of the Conformation-Specific IR Spectra of Ethyl, *n*-Propyl, and *n*-Butylbenzene, *J. Chem. Phys.* **144**, 224310 (2016). DOI: 10.1063/1.4953181

7. E.L. Sibert III, **D.P. Tabor**, and J.M. Lisy, Modeling The CH Stretch Vibrational Spectroscopy of M^+[Cyclohexane] (M=Li, Na, and K) Ions, *J. Phys. Chem. A* **119**, 10293-10299 (2015). DOI: 10.1021/acs.jpca.5b07461 (ACS Editors' Choice).

6. **D.P. Tabor**, R. Kusaka, P.S. Walsh, T.S. Zwier, and E.L. Sibert III, Local Mode Approach to OH Stretch Spectra of Benzene-$(H_2O)_n$ Clusters, $n = 2-7$, *J. Phys. Chem. A* **119**, 9917-9930 (2015). DOI: 10.1021/acs.jpca.5b06954

5. **D.P. Tabor**, R. Kusaka, P.S. Walsh, E.L. Sibert III, and T.S. Zwier, Isomer-Specific Spectroscopy of Benzene-$(H_2O)_n$, $n = 6,7$: Benzene's Role in Re-Shaping Water's Three-Dimensional Networks, *J. Phys. Chem. Lett.* **6**, 1989-1995 (2015). DOI: 10.1021/acs.jpclett.5b00786

4. Y.-F. Lee, W.-T. Chou, B.A. Johnson, **D.P. Tabor**, E.L. Sibert III, and Y.-P. Lee , Infrared Absorption of CH_3O and CD_3O Radicals Isolated in Solid Para-H_2, *J. Mol. Spectrosc.* **310**, 57-67 (2015). DOI: 10.1016/j.jms.2014.11.008

3. E.L. Sibert III, **D.P. Tabor**, N.M. Kidwell, J.C. Dean, and T.S. Zwier, Fermi Resonance Effects in the Vibrational Spectroscopy of Methyl and Methoxy Groups, *J. Phys. Chem. A* **118**, 11272-11281 (2014). DOI: 10.1021/jp510142g

2. E.L. Sibert III and **D.P. Tabor**, A Perturbative Description of Non-Adiabatic Effects in Methoxy Vibrations, *Mol. Phys.* **112**, 3138-3143 (2014). DOI: 10.1080/00268976.2014.932455

1. **D.P. Tabor**, M.E. Harding, T. Ichino, and J.F. Stanton, High Accuracy Extrapolated Ab Initio Thermochemistry of the Vinyl, Allyl, and Vinoxy Radicals, *J. Phys. Chem. A* **116**, 7668-7676 (2012). DOI: 10.1021/jp302527n

Technical Reports

1. Materials Acceleration Platform: Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods with Artificial Intelligence (co-author). View at: link

Funding Obtained in Independent Career

Budgeted Tabor Group Portion Indicated on Multi-Investigator Grants.

Current

Robert A. Welch Foundation 06/01/2026-05/31/2029 $351,000
Grant No. A-2049-20260402
Title: Accelerating Computational Spectroscopy Prediction and Analysis with Physically Motivated Machine Learning Methods
Principal Investigator

Research Corporation for Science Advancement 07/01/2026-06/30/2027 $66,000
Scialog Automating Chemical Laboratories Seed Grant
Grant No. SA-AUT-2026-079B
Title: Temporally Adaptive Design of Organic Flow Battery Systems
Principal Investigator
Co-PI: Cailin Buchanan (Argonne National Laboratory)

Research Corporation for Science Advancement 07/01/2025-06/30/2027 $66,000
Scialog Automating Chemical Laboratories Seed Grant
Grant No. SA-AUT-2025-037b
Title: Breaking the Polymer Bottleneck: In-Line High-Throughput Nanoprecipitation
Principal Investigator
Co-PI: Emily Davidson (Princeton University), Melody Morris (UMass-Amherst)

Sandia National Laboratories 12/2023-09/2026 $ 179,550
Sandia LDRD Program
Title: Cryptand Molecular Cavities to Capture and Chemically Process CO_2
Co-PI (PI: Timothy S. Zwier, Sandia National Laboratory)

National Science Foundation 12/15/2023-11/30/2028 $ 625,000
NSF Award Number: 2339804
Title: CAREER: Development of Adaptive and Efficient Computational Inverse Design Methods for Organic Functional Materials
Principal Investigator

National Science Foundation 10/01/2023-09/30/2028 $ 327,242
NSF Award Number: 2303044 (Estimated Group Portion)
Title: NSF Center for the Mechanical Control of Chemistry (Phase II)
PI: James Batteas
All other investigators in a CCI are Senior Personnel

Research Corporation for Science Advancement 07/01/2023-06/30/2026 $100,000
Cottrell Scholar Program
Grant No. CS-CSA-2023-054
Title: Intelligent Optimization of Organic Photophysical Chemical Spaces
Principal Investigator

Former

Kureha Corporation 1/1/2024-6/30/2025 $ 170,460
Principal Investigator

Robert A. Welch Foundation 06/01/2023-05/31/2026 $300,000
Grant No. A-2049-20230405
Title: Accelerating the Prediction and Analysis of Vibrational and Electronic Spectroscopy
Principal Investigator

National Science Foundation 10/01/2021-03/31/2026 $429,587
Grant No. DMR-2119672 (Estimated Group Portion)
Title: Collaborative Research: DMREF: Accelerated Design of Redox-Active Polymers for Metal-Free Batteries
(Co-PI with Jodie Lutkenhaus (lead), Juan de Pablo, and Stuart Rowan)

National Science Foundation 08/09/2019-08/31/2023 $70,000
Grant CMMI-1930277
Data Science Supplement to: Cellulose Nanocrystal-enabled Manufacturing of Carbon Nanotube Carbon fiber Polymer Composites
(Subcontract for Data Science Supplement. PIs: Amir Asadi, Lisa Perez)

Robert A. Welch Foundation 06/01/2020-05/31/2023 $240,000
Grant No. A-2049-20200401
Title: Mapping the Structure and Formation of Aerosols Through Theoretical Spectroscopy and Multiscale Simulation
Principal Investigator

Texas A&M T3: Triads for Transformation 01/01/2020-12/31/2021 $10,000
Closed-Loop Discovery Of Radical Biopolymers For Organic Battery Electrodes
(Co-PI with Karen Wooley and Jodie Lutkenhaus)

Texas A&M Institute for Data Science: Data Science Career Initiation Fellow Program 05/01/2021-12/31/2022 $10,000
Title: Scientific Machine Learning for Chemical Physics Based Materials Design
Principal Investigator

Honors and Awards

During Independent Career

2025 Journal of Physical Chemistry C Lectureship Award, PHYS Division, ACS

2024 ACS COMP Division Cadence/OpenEye Award for Junior Faculty

2024 Finalist for ACS Energy Letters Early Career Lectureship for Energy Storage

2024 Scialog Fellow for Automating Chemical Laboratories (Research Corporation for Science Advancement)

2023 Montague-Texas A&M Center for Teaching Excellence Scholar Award

2023 Cottrell Scholar (Research Corporation for Science Advancement)

2021 Texas A&M Institute for Data Science Career Initiation Fellow

Prior to Independent Career

2016 Richard and Joan Hartl Excellence in Research Award for Physical Chemistry, University of Wisconsin–Madison

2015 Poster Award, Physical Division, ACS National Meeting, Boston, Massachusetts

2015 Poster Award, Midwest Theoretical Chemistry Conference, Ann Arbor, Michigan

2013 Department of Chemistry Outstanding Teaching Assistant Award, University of Wisconsin–Madison

2011 Hirschfelder Graduate Fellowship, University of Wisconsin–Madison

2010-2011 Beckman Scholar

Presentations

Invited Seminars, Independent Career

1. University of Massachusetts–Amherst, May 2025.
2. University of Illinois Urbana-Champaign Department of Chemistry, April 2025.
3. University of California–Irvine Department of Chemistry, April 2025.
4. University of Florida Department of Chemistry, April 2025.
5. University of Maryland Department of Chemistry, March 2025.
6. Emory University Department of Chemistry, February 2025.
7. Georgia Tech Department of Chemistry, February 2025.
8. Princeton University Department of Chemistry, February 2025.
9. University of California–San Diego Department of Chemistry, January 2025.
10. Southern Utah University Department of Chemistry, November 2024.
11. University of Washington Department of Chemistry, October 2024.
12. University of Buffalo Department of Chemical and Biological Engineering, September 2024.

13. University of Memphis Department of Chemistry, September 2024.
14. Yale University Department of Chemistry, April 2024.
15. Stony Brook University Department of Chemistry, April 2024.
16. University of Wisconsin–Madison Department of Chemistry, April 2024.
17. University of Oklahoma Department of Chemistry, March 2024.
18. Johns Hopkins University Department of Chemistry, March 2024.
19. University of Texas at Austin Department of Chemistry, February 2024.
20. University of Kentucky Department of Chemistry, November 2023.
21. University of Utah Department of Chemistry, October 2023.
22. Louisiana State University Department of Chemistry, April 2023.
23. Southern Methodist University Department of Chemistry, March 2023.
24. University of Mississippi Department of Chemistry, March 2023.
25. Texas A&M University–Kingsville Department of Chemistry, October 2022.
26. Duquesne University Department of Chemistry and Biochemistry, September 2022.
27. Los Alamos National Laboratory Theoretical Division and Center for Integrated Nanotechnologies (CINT), April 2022.
28. University of California-Merced Department of Chemistry and Biochemistry, April 2022.
29. University of Florida Theoretical Group Virtual Seminar Series. February 2021. Virtual talk given on Zoom.

Invited Talks, Independent Career

30. Identifying Promising Mechanochemical Reactions Through High-Throughput Virtual Screening, Machine Learning, and Simplified Physical Models, 11th International Conference on Mechanochemistry and Mechanical Alloying (INCOME), September 2025, Berlin, Germany.
31. Accelerating the computational design of functional organic molecules and polymers, 270^{th} ACS National Meeting. PHYS Division, August 2025, Washington, DC. (JPC C Lectureship Talk).
32. Accelerating energy storage materials design with the integration of multiscale simulations and machine learning, 270^{th} ACS National Meeting. Energy and Fuels Division, August 2025, Washington, DC.
33. Identifying Mechanochemically Accelerated Reactions, Center for the Mechanical Control of Chemistry Discussions, April 2025 (Talk Given on YouTube)
34. Inverse Organic Materials Design with Reinforcement Learning, 268^{th} ACS National Meeting. Computers in Chemistry Division, August 2024, Denver, CO. (ACS COMP Award Symposium Talk)
35. Developing Machine Learning Methods for Accelerating Energy Storage Materials Design and Simulation, 268^{th} ACS National Meeting. Energy and Fuels Division, August 2024, Denver, CO. (ACS ENFL Award Symposium Talk)
36. Combining Physics-Based and Data-Driven Models for Accelerating Condensed Phase Spectroscopy Simulations, 267^{th} ACS National Meeting. Physical Chemistry Division, March 2024, New Orleans, LA.

37. Machine-learning-driven approaches for organic electronic materials discovery and design, 266^{th} ACS National Meeting. Physical Chemistry Division, August 2023, San Francisco, CA.
38. Data-driven methods for accelerating condensed phase vibrational spectroscopy modeling, 265^{th} ACS National Meeting. Physical Chemistry Division, March 2023, Indianapolis, IN.
39. Data-Driven Methods for Accelerating Vibrational Spectroscopy Modeling at the Medium to Large Scale, Texas A&M High-Performance Research Computing Conference. May 2022. College Station, TX.
40. Data-Driven Methods for Accelerating Vibrational Spectroscopy Modeling at the Medium to Large Scale, ACS Southwest Regional Meeting. October 2021. Austin, TX.
41. Active Search for Organic Functional Materials with Machine Learning, Southwest Theoretical and Computational Chemistry Meeting. October, 2019. Norman, OK.

Contributed Talks, Independent Career

42. Optimizing Conformer-specific Spectral Assignments with an Adaptive and Automated Approach, 78^{th} International Symposium on Molecular Spectroscopy, June 2025, Urbana, IL.
43. Using Machine Learning To Generate Molecules With Desired Spectroscopic Features, 77^{th} International Symposium on Molecular Spectroscopy, June 2024, Urbana, IL.
44. Leveraging Fragment-Based Representations in Active Learning and Reinforcement Learning Frameworks for Materials Design, MRS Spring Meeting, April 2023, Seattle, WA.
45. Coupling Reinforcement Learning Approaches with Efficient Quantum Chemical Models for Organic Electronic Materials Discovery and Design, MRS Fall Meeting, November 2023, Boston, MA.
46. Learning Molecular Hamiltonians Directly from Spectra, 76^{th} International Symposium on Molecular Spectroscopy, June 2023, Urbana, IL.
47. Assigning the vibrational spectra of clusters directly from the spectrum, 265^{th} ACS National Meeting. Physical Chemistry Division, March 2023, Indianapolis, IN.
48. Developing Physically Motivated, Data-Driven Models for the Accurate Prediction of Disordered Protein Polymer Physics, 265^{th} ACS National Meeting. Computers in Chemistry Division, March 2023, Indianapolis, IN.
49. Multiscale Simulation and Computational Design of Non-Conjugated Radical Polymers for Energy Storage Applications, 264^{th} ACS National Meeting. Polymeric Materials: Science and Engineering Division, August 2022, Chicago, IL.
50. Inverse Infrared Spectroscopy via a Data-Driven Approach, 264^{th} ACS National Meeting. Computers in Chemistry Division, August 2022, Chicago, IL.
51. Identification of the key molecular and polymeric levers for maximizing the conductivity of non-conjugated radical polymers via molecular simulation, 263^{rd} ACS National Meeting. Physical Division, March 2022, San Diego, CA.
52. Data-Driven Methods for Accelerating Vibrational Spectroscopy Modeling at the Medium to Large Scale, Sanibel Symposium. February 2022. St. Simon's Island, GA. (Hot-topic talk)
53. Structure and Infrared Spectra of New Aerosol Particle Formation Seed Clusters, 74^{th} International Symposium on Molecular Spectroscopy. June 2021 (Virtual Talk).
54. Theoretical models and computational design of conductive non-conjugated radical polymers for energy storage, 261^{st} ACS National Meeting. Computers in Chemistry Division, April 2021 (Virtual Talk).

55. Active Multi-objective Search for High-performance Organic Functional Materials, 2020 Prairie View A&M/Texas A&M Joint Data Blitz Symposium, Feb. 2020. Prairie View, TX.

Poster Presentations, Independent Career

56. Optimizing Mechanochemical Reaction Acceleration via Active Search, Sanibel Symposium. February 2025, St. Augustine, FL.
57. Accelerating Molecular Interaction and Spectroscopy Modeling with Machine Learning, Gordon Research Conference on Molecular Interactions and Dynamics. July 2024, Stonehill, MA. (Selected for short talk).
58. Data-Driven Methods for Accelerating Condensed Phase Vibrational Spectroscopy Modeling, Gordon Research Conference on Liquids. July 2023, Holderness, NH.
59. Active, Multi-Objective Search for Organic Energy Storage Materials, Virtual Conference on Theoretical Chemistry. July 2020. Virtual Conference held in place of the American Conference on Theoretical Chemistry.

Invited Talks, Prior to Independent Career

1. Flow Battery Electrolyte Discovery, JCESR Redoxmer Workshop, May 2019. Boston, MA.
2. Organic Functional Materials Discovery: The Importance of New Optimization Algorithms, 257^{th} ACS National Meeting. Computers in Chemistry Division. March 2019. Orlando, FL
3. Organic Flow Battery Electrolyte Discovery: Importance of New Optimization Algorithms, European Energy Research Alliance Autonomous Materials Development Platforms Workshop. October 2018. Brussels, Belgium.
4. Accelerated Discovery of Materials for Organic Redox Flow Batteries, Mission Innovation Business Day. May 2018. Malmö, Sweden.
5. Modeling Vibrational Spectra with a Local Mode Approach, University of Wisconsin-Madison Departmental Awards Seminar. May 2016. Madison, WI.

Contributed Talks, Prior to Independent Career

6. Discovery of Organic Flow Battery Electrolytes via a Machine Learning Driven Approach, 256^{th} ACS National Meeting. Energy and Fuels Division. August 2018. Boston, MA.
7. Coupling Generative Models to Virtual Screening: Application to Organic Redox Flow Batteries, 255^{th} ACS National Meeting. Computers in Chemistry Division. March 2018. New Orleans, LA.
8. Influence of Aromatic Molecules on The Structure and Spectroscopy of Water Clusters, 71^{st} International Symposium on Molecular Spectroscopy. June 2016. Urbana, IL.
9. Modeling the Conformation-Specific Infrared Spectroscopy of N-Alkylbenzenes, 71^{st} International Symposium on Molecular Spectroscopy. June 2016. Urbana, IL
10. Theoretical Study of the IR Spectroscopy of Benzene-$(Water)_n$ Clusters, 70^{th} International Symposium on Molecular Spectroscopy. June 2015. Urbana, IL.
11. Vibrational Spectroscopy of Benzene-$(Water)_n$ Clusters with $n = 6, 7$, 70^{th} International Symposium on Molecular Spectroscopy. June 2015. Urbana, IL.
12. Theoretical Study of the Ethyl Radical, 69^{th} International Symposium on Molecular Spectroscopy. June 2014. Urbana, IL.

13. Theoretical Study of the Ethyl Radical, 68^{th} International Symposium on Molecular Spectroscopy. June 2013. Columbus, OH.

Poster Presentations, Prior to Independent Career

14. Accelerating the Rate of Discovery of Organic Functional Materials, Flatiron Institute Center for Computational Quantum Physics Quantum Chemistry Workshop. November 2017. New York, NY.
15. High-Throughput Virtual Screening of Flow Battery Electrolytes, American Conference on Theoretical Chemistry. July 2017. Boston, MA.
16. High-Throughput Virtual Screening of Flow Battery Electrolytes, MIT Energy Night. October 2016. Cambridge, MA.
17. Theoretical Study of the IR Spectroscopy of Benzene-(Water)$_n$ Clusters with $n = 3-7$, 250^{th}ACS National Meeting. Physical Division. August 2015. Boston, MA.
18. Theoretical Study of the IR Spectroscopy of Benzene-(Water)$_n$ Clusters with $n = 3-7$, Midwest Theoretical Chemistry Conference. June 2015. Ann Arbor, MI.
19. Probing Molecular Structure with CH Chromophores" Gordon Research Conference on Vibrational Spectroscopy. August 2012. Biddeford, ME.
20. Towards a Potential Energy Surface for Vibrational Analysis of the Ethyl Radical, Midwest Theoretical Chemistry Conference. June 2012. Madison, WI.
21. Computing Highly Accurate Enthalpies of Formation via Isodesmic and Hypohomodesmotic Schemes, Beckman Research Symposium. August 2011. Irvine, CA.
22. Computing Highly Accurate Enthalpies of Formation via Isodesmic and Hypohomodesmotic Schemes, Dynamics of Molecular Collisions Conference. July 2011. Snowbird, UT.

Teaching and Mentoring

Teaching

Courses Taught

Spring 2026 HONR 102: Seminar in Loyalty, Integrity, and Selfless Service

Fall 2025, Fall 2026 HONR 101: Seminar in Respect, Excellence and Leadership

Fall 2021, Fall 2022, Fall 2023, Fall 2024, Fall 2025, Fall 2026 Chemistry 119H (Honors Fundamentals of Chemistry I)

Fall 2020, Fall 2021, Fall 2025 Chemistry 631 (Statistical Thermodynamics Graduate Level)

Fall 2019, Fall 2020, Fall 2022, Fall 2023 Chemistry 648 (Principles of Quantum Mechanics Graduate Level)

Mentoring

Current Graduate Students

2025- Partha Dash

2024- Eden Brenneman

2024- Hao Zhan

2024- Yeu-Shiuan (Sharon) Ho

2022- Hayden Moran

2023 NDSEG Fellow

2021- Tzu-Hsuan Chao

2020- Abigail Moody

Current Postdoctoral Fellows

2026- Saikiran Kotaru

2025- Nicholas Hopper

2024- Mark Boyer

Current Undergraduate Students

2026- Alexander Entchev

2025- Emily Padilla

2025- Aidan Chance

2025- Jackson Schwedler

Former Group Members

Graduate Students

Cheng-Han Li (2024 Ph.D.)

Katie Felde (2025 M.S.)

Daniel Doria (2025 M.S.)

Jezrielle Annis (2024 M.S.)

Postdoctoral Fellows

2020-2022 Shi Li

Now at Argonne National Laboratory

2023-2026 Vijay Sundar

Undergraduates

2025-2026 John Elmore

2025-2026 Shaili Ghandi

2024-2025 William Colglazier

2024 Tanya Chandra

2022-2024 David Chi

2020-2024 Curran Watson

Current Ph.D. student in chemistry, Virginia Tech

2024 Manasi Ramkumar

2023 Autumn Kimber

2023 Alejandro Mejias

2023 Fernando Ramirez

2022-23 Samantha Rosal

Current Ph.D. student in computational chemistry, Washington University St. Louis

2022-2023 Jae Trinh

2022 Avi Bedi (2022 REU Student from Butler University)

2021-2022 Zachary Graham

2021 Daniel Hernandez

2021 Tyler Paxton

2021 Logan Hendricks

2021 David A. González Narváez (2021 Chemistry Department NSF REU Student)

Current Ph.D. student in theoretical chemistry, Columbia University

2021 Olivia McNally (NSF REU Student, co-advised with Prof. Emily Pentzer)

2021 Brittany DeNicholas (NSF REU Student, co-advised with Prof. Emily Pentzer)

2021 Jia Li (2021 REU Student, co-advised with Prof. Amir Asadi)

2020-2021 Emily Chappie (Remote Visiting Scholar from the Kidwell Group at William & Mary)

Current: OpenEye

2020-2022 Brianna Bishop

2021 Goldwater Scholar

Service

University and Department Service

2021- Director, Undergraduate Chemistry Honors Program

2025- Departmental Graduate Awards Committee

2024- Departmental Undergraduate Curriculum Commitee

2022-2024 Department of Chemistry Graduate Admissions Committee Member

2022-2024 Chair of Texas A&M Local ACS Section

2022-2023 Elevating Honors Advisory Committee Member

2022- Facilitator for Texas A&M Graduate Mentoring Academy

2021 College of Science Information Technology Director Search Committee Member

2021 Laboratory for Molecular Simulation Research Scientist Search Committee Member

2019-2022, 2023-2024 Faculty Candidate Search Committee Member

2020 Hullabaloo U Instructor

2020-2024 Department Proactive Recruiting Operations (PROps) Committee Member

2019-2023 Department Information Technology Committee Member

Scientific Committees and Professional Activities

2025 Mail-in Reviewer for National Science Foundation

2024 Reviewer for Department of Energy

2024 Reviewer for Research Corporation for Science Advancement

2024 Reviewer for ACS PRF

2024 Reviewer for National Science Foundation

2023 Miller Prize Judge for International Symposium for Molecular Spectroscopy

2023 Reviewer for Research Corporation for Science Advancement

2023 Reviewer for ACS COMP Division Award

2022-2023 Co-editor (with Zhou Lin) of Special Issue on Machine Learning in Spectroscopy for the Journal of Molecular Spectroscopy

2022 Poster Session Judge for Physical Division at Spring 2022 ACS Meeting

2022 Mail-in Reviewer for U.S. Department of Energy

2022 Reviewer for TAMU Qatar Proposals

2022 Co-organizer (with Kelvin Lee) of the Machine Learning in Spectroscopy Minisymposium at the International Symposium for Molecular Spectroscopy

2021 Mail-in Reviewer for U.S. Department of Energy

2021 Panel Reviewer and ad hoc Reviewer for National Science Foundation

2020 Participant, JCESR ML/AI Virtual Workshops

2019 Invited Participant, NSF Summit on Big Data and Cyberinfrastruture for Materials Research, Chicago, Illinois

2019 Panel Reviewer for U.S. Department of Energy

2019 Participant, Cottrell Scholars Collaborative/ACS New Faculty Workshop, Pasadena, CA

2018 Panel Reviewer: Sectoral Fund CONACYT-Secretariat of Energy-Energy Sustainability, Mexico

2018 Invited Participant, ARPA-E Machine Learning Workshop, Falls View, Virginia

2017 Participant, Mission Innovation Clean Energy Materials Innovation Challenge Workshop, Mexico City, Mexico

Scientific Refereeing of Publications

Referee: *ACS Appl. Polym. Mater., ACS Cent. Sci., ACS Omega, Adv. Mater., Adv. Theor. Sim., Angew. Chem., Batter. Supercaps, Cell Rep. Phys. Sci., Chem. Mater., Chem. Sci., Digital Discovery, Energy Env. Sci., J. Am. Chem. Soc., J. Mater. Chem. A, J. Phys. Chem. A, J. Phys. Chem. C, Joule, Mater. Horiz., Mol. Phys., Nanoscale Horiz., Nat. Energy, Phys. Chem. Chem. Phys., RSC Adv., Trends Chem.* (90 total manuscripts since starting independent career)

2024 Named Outstanding Reviewer for Digital Discovery

Outreach and Related Activities

2024 Volunteer for Texas A&M Chemistry Department High School Summer Outreach Programs and Demonstrations

2023-2025 Volunteer for Texas A&M Chemistry Department High School Outreach Events at Rudder High School in Bryan, TX

2022 Texas A&M Institute for Data Science FAIR Data Science Virtual Workshop (co-organized with Lauren Sare and John Watts, 2 workshops)

2021-2024 Texas A&M Department of Chemistry Open House Demos

Professional Society Memberships

2009- Member, American Chemical Society