ROBERT B. WEXLER

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EDUCATION

Ph.D. in Chemistry, University of Pennsylvania, Philadelphia, PA 2019
Advisor: Andrew M. Rappe

B.S. (first honors) in Chemistry, Drexel University, Philadelphia, PA 2013
Minor in Music

PROFESSIONAL POSITIONS

Assistant Professor of Chemistry 2022 - present
Washington University in St. Louis *St. Louis, MO*

Postdoctoral Research Associate in Mechanical and Aerospace Engineering 2019 - 2022
Princeton University *Princeton, NJ*
Advisor: Emily A. Carter

RESEARCH ACTIVITIES

Theoretical materials innovation for renewable energy and environmental applications, with a particular emphasis on developing computational methods for the more realistic modeling of interfacial phenomena in electrocatalysis, solar energy conversion, and environmental energy harvesting

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Google Scholar: https://scholar.google.com/citations?user=BMnroAsAAAAJ&hl=en&oi=ao

GitHub: https://github.com/wexlergroup

AWARDS AND HONORS

- 2017 Award for Excellence in Chemistry Graduate Research, UPenn
- 2016 Departmental Fellowship, UPenn
- 2015 Teaching Assistant Award, UPenn
- 2013 William Fontaine Fellowship, UPenn
- 2013 HyperCube Scholar Award, Drexel
- 2013 American Institute of Chemists Baccalaureate Award, Drexel

MEMBERSHIPS IN PROFESSIONAL SOCIETIES

- American Chemical Society (2013 - present)
- American Physical Society (2013 - present)
- American Institute of Chemical Engineers (2019 - present)

REFEREE SERVICES TO SCHOLARLY PUBLICATIONS

ACS Catalysis, ACS Central Science, ACS Materials Letters, Applied Physics A, Catalysts, Chemistry of Materials, Computer Physics Communications, Energy & Environmental Science, Energy Technology, Journal of Physical Chemistry, Journal of Applied Physics, Journal of the American Chemical Society, Journal of the Electrochemical Society, Minerals, Molecules, Nanoscale, Nature Communications, Nature Computational Science, npj Computational Materials, Physical Chemistry Chemical Physics, Physical Review Applied, Physical Review B, Physical Review Letters, Physical Review Materials, Physical Review Research, and RSC Advances

PROFESSIONAL/COMMUNITY SERVICE

- AACT/ACS Science Coaches Program (2023 - present)
- Symposium Organizer, "Chemical Theory Across Scales," Joint Midwest & Great Lakes Regional Meeting (2023)
- Organizer, "Summer of Chemical Theory" (2023 - present)
- Letters to a Pre-Scientist (2020 - present)
- Skype a Scientist (2020 - present)
- Session Chair, "Computational Design and Discovery of Novel Materials," APS March Meeting (2022)

LIST OF PUBLICATIONS

23. M. Yang, L. B. Pártay, and R. B. Wexler, "Surface phase diagrams from nested sampling," *Phys. Chem. Chem. Phys.*, **Advance Article** (2024).
https://doi.org/10.1039/D4CP00050A

22. K. Choudhary, D. Wines, K. Li, K. F. Garrity, V. Gupta, A. H. Romero, J. T. Krogel, K. Saritas, A. Fuhr, P. Ganesh, P. R. C. Kent, K. Yan, Y. Lin, S. Ji, B. Blaiszik, P. Reiser, P. Friederich, A. Agrawal, P. Tiwary, E. Beyerle, P. Minch, T. D. Rhone, I. Takeuchi, R. B. Wexler, A. Mannodi-Kanakkithodi, E. Ertekin, A. Mishra, N. Mathew, S. G. Baird, M. Wood, A. D. Rohskopf, J. Hattrick-Simpers, S.-H. Wang, L. E. K. Achenie, H. Xin, M. Williams, A. J. Biacchi, and F. Tavazza, "Large Scale Benchmark of Materials Design Methods," *accepted.*
https://doi.org/10.48550/arXiv.2306.11688

Before WashU

21. E. Lupi, R. B. Wexler, D. Meyers, A. Zahradnik, Y. Jiang, S. Susarla, R. Ramesh, L. W. Martin, and A. M. Rappe, "Engineering Relaxor Behavior in $(BaTiO_3)_n/(SrTiO_3)_n$ Superlattices," *Adv. Mater.*, **35**, 2302012 (2023).
https://doi.org/10.1002/adma.202302012

20. R. B. Wexler, E. B. Stechel, and E. A. Carter, "Materials Design Directions for Solar Thermochemical Water Splitting," in *Solar Fuels*, Vol. 3, Nurdan Demirci Sankir & Mehmet Sankir, Eds. (Wiley-Scrivener, USA), in press (2023).
https://doi.org/10.1002/9781119752097.ch1

19. R. B. Wexler and E. A. Carter, "Oxygen-Chlorine Chemisorption Scaling for Seawater Electrolysis on Transition Metals: The Role of Redox," *Adv. Theory Simul.*, **6**, 2200592 (2023).
https://doi.org/10.1002/adts.202200592

18. S. Banerjee, A. Kakekhani, R. B. Wexler, and A. M. Rappe, "Relationship between the Surface Reconstruction of Nickel Phosphides and Their Activity toward the Hydrogen Evolution Reaction," *ACS Catal.*, **13**, 4611 (2023).
https://doi.org/10.1021/acscatal.2c06427

17. L. Gao, R. B. Wexler, R. Fei, and A. M. Rappe, "Ab Initio Study of Hydrogen Niobate $HNbO_3$: Structural, Thermodynamic, Dielectric, and Optical Properties," *J. Phys. Chem. C*, **127**, 5931 (2023).
https://doi.org/10.1021/acs.jpcc.2c07844

16. R. B. Wexler, G. S. Gautam, R. T. Bell, S. Shulda, N. A. Strange, J. A. Trindell, J. D. Sugar, E. Nygren, S. Sainio, A. H. McDaniel, D. Ginley, E. A. Carter, and E. B. Stechel, "Multiple and nonlocal cation redox in Ca–Ce–Ti–Mn oxide perovskites for solar thermochemical applications," *Energy Environ. Sci.*, **16**, 2550 (2023).
https://doi.org/10.1039/D3EE00234A

15. S. Banerjee, A. Kakekhani, R. B. Wexler, and A. M. Rappe, "Mechanistic Insights into CO_2 Electroreduction on Ni_2P: Understanding Its Selectivity toward Multicarbon Products," *ACS Catal.*, **11**, 11706 (2021).
https://doi.org/10.1021/acscatal.1c03639

14. R. B. Wexler, G. S. Gautam, E. B. Stechel, and E. A. Carter, "Factors Governing Oxygen Vacancy Formation in Oxide Perovskites," *J. Am. Chem. Soc.*, **143**, 13212 (2021).
https://doi.org/10.1021/jacs.1c05570

13. Y.-H. Kim, S. Kim, A. Kakekhani, J. Park, J. Park, Y.-H. Lee, H. Xu, S. Nagane, R. B. Wexler, D.-H. Kim, S. H. Jo, L. Martínez-Sarti, P. Tan, A. Sadhanala, G.-S. Park, Y.-W. Kim, B. Hu, H. J. Bolink, S. Yoo, R. H. Friend, A. M. Rappe, and T.-W. Lee, "Comprehensive defect suppression in perovskite nanocrystals for high-efficiency light-emitting diodes," *Nat. Photonics*, **15**, 148 (2021).
https://doi.org/10.1038/s41566-020-00732-4

12. R. B. Wexler, G. S. Gautam, and E. A. Carter, "Optimizing kesterite solar cells from Cu_2ZnSnS_4 to $Cu_2CdGe(S,Se)_4$," *J. Mater. Chem. A*, **9**, 9882 (2021).
https://doi.org/10.1039/D0TA11603C

11. R. B. Wexler, G. S. Gautam, and E. A. Carter, "Exchange-correlation functional challenges in modeling quaternary chalcogenides," *Phys. Rev. B*, **102**, 054101 (2020).
https://doi.org/10.1103/PhysRevB.102.054101

Before Princeton

10. R. B. Wexler, Y. Qi, and A. M. Rappe, "Sr-induced dipole scatter in $Ba_xSr_{1-x}TiO_3$: Insights from a transferable-bond valence-based interatomic potential," *Phys. Rev. B*, **100**, 174109 (2019).
https://doi.org/10.1103/PhysRevB.100.174109

9. R. B. Wexler, T. Qiu, and A. M. Rappe, "Automatic Prediction of Surface Phase Diagrams Using Ab Initio Grand Canonical Monte Carlo," *J. Phys. Chem. C*, **123**, 2321 (2019).
https://doi.org/10.1021/acs.jpcc.8b11093

8. A. B. Laursen, R. B. Wexler, M. J. Whitaker, E. J. Izett, K. U. D. Calvinho, S. Hwang, R. Rucker, H. Wang, J. Li, E. Garfunkel, M. Greenblatt, A. M. Rappe, and G. C. Dismukes, "Climbing the Volcano of Electrocatalytic Activity while Avoiding Catalyst Corrosion: Ni_3P, a Hydrogen Evolution Electrocatalyst Stable in Both Acid and Alkali", *ACS Catal.*, **8**, 4408 (2018).
https://doi.org/10.1021/acscatal.7b04466

7. R. B. Wexler, J. M. P. Martirez, and A. M. Rappe, "Chemical Pressure-Driven Enhancement of the Hydrogen Evolving Activity of Ni_2P from Nonmetal Surface Doping Interpreted via Machine Learning," *J. Am. Chem. Soc.*, **140**, 4678 (2018).
https://doi.org/10.1021/jacs.8b00947

6. R. B. Wexler, J. M. P. Martirez, and A. M. Rappe, "Active Role of Phosphorus in the Hydrogen Evolving Activity of Nickel Phosphide (0001) Surfaces," *ACS Catal.*, **7**, 7718 (2017).
https://doi.org/10.1021/acscatal.7b02761

5. C. H. Naylor, W. M. Parkin, Z. Gao, H. Kang, M. Noyan, R. B. Wexler, L. Z. Tan, Y. Kim, C. E. Kehayias, F. Streller, Y. R. Zhou, R. Carpick, Z. Luo, Y. W. Park, A. M. Rappe, M. Drndić, J. M. Kikkawa, and A. T. C. Johnson, "Large-area synthesis of high-quality monolayer 1T'-WTe_2 flakes," *2D Mater.*, **4**, 021008 (2017).
https://doi.org/10.1088/2053-1583/aa5921

4. R. B. Wexler, J. M. P. Martirez, and A. M. Rappe, "Stable Phosphorus-Enriched (0001) Surfaces of Nickel Phosphides," *Chem. Mater.*, **28**, 5365 (2016).
https://doi.org/10.1021/acs.chemmater.6b01437

3. R. B. Wexler and K. Sohlberg, "Models for the Temperature and Gas Partial Pressure Dependence of Conductance," *Rev. Theor. Sci.*, **4**, 97 (2016).
https://doi.org/10.1166/rits.2016.1051

2. R. B. Wexler and K. Sohlberg, "Role of Proton Hopping in Surface Charge Transport on Tin Dioxide As Revealed by the Thermal Dependence of Conductance," *J. Phys. Chem. A.*, **118**, 12031 (2014).
https://doi.org/10.1021/jp5076719

1. F. Levine, R. V. Kayea III, R. B. Wexler, D. J. Sadvary, C. Melick, and J. La Scala, "Heats of Combustion of Fatty Acids and Fatty Acid Esters," *J. Am. Oil Chem. Soc.*, **91**, 235 (2013).
https://doi.org/10.1007/s11746-013-2367-0

PATENTS

- Emily A. Carter, Robert B. Wexler, Sai Gautam Gopalakrishnan, and Ellen B. Stechel, *Perovskites for reduction-re-oxidation thermochemical water and carbon dioxide splitting.* Patent application US20230357046A1. Published Nov. 9, 2023.
  https://patents.google.com/patent/US20230357046A1/en
- Emily A. Carter, Robert B. Wexler, and Sai Gautam Gopalakrishnan, *$Cu_2CdGe(S, Se)_4$ Solar Cell Absorbers.* Patent application US20230268451A1. Filed Jul. 24, 2020.
  https://patents.google.com/patent/US20230268451A1/en

SEMINARS AND PRESENTATIONS

A. Invited Seminars

5. Sep. 11, 2023: "Methods To Model the Imperfections of Materials," Department of Chemistry, Murray State University, Murray, KY
4. Sep. 7, 2023: "Surface Phase Diagrams From Nested Sampling," Department of Physics, Washington University in St. Louis, St. Louis, MO.
3. Sep. 12, 2022: "Computational Materials Design for Sustainable Energy Technologies," Institute of Materials Science & Engineering, Washington University in St. Louis, St. Louis, MO.
2. Sep. 13, 2021: "Data-Driven Computational Materials Design for Sustainable Energy Technologies," Department of Chemistry, University of Iowa, Iowa City, IA (virtual).
1. Oct. 9, 2020: "Computational Design of Sustainable Energy Materials: From Quantum Mechanics to Machine Learning," Department of Chemistry, Drexel University, Philadelphia, PA (virtual).

B. Invited Talks

8. May 30 – June 1, 2024: Invited talk at the 54th Midwest Theoretical Chemistry Conference.
7. Mar. 18, 2024: "$(Ca, Ce)(Ti, Mn)O_3$ Perovskites for Two-Step Solar Thermochemical H_2 Production," *Fundamentals to Applications – Advances in material-based hydrogen storage for energy and industry at the ACS Spring 2024*, New Orleans, LA.
6. Feb. 20, 2024: "Predicting the Equilibrium Structure of Catalyst Surfaces With Nested Sampling," *Inaugural Workshop of the Initiative for Computational Catalysis*, Flatiron Institute, New York, NY.
5. Sep. 13, 2023: "Modeling-Driven Design of Redox-Active Off-Stoichiometric Oxides for Solar Thermochemical Water Splitting," *International Forum on Hydrogen Production Technologies* (virtual).
4. Aug. 16, 2023: "Path of Least Resistance: Predictive Thermochemical Cycles for Bulk and Surface Catalysis," *Data Science for Catalysis: Structural Evolution, Reaction Kinetics, and Catalysis Informatics at the ACS Fall 2023*, San Francisco, CA.
3. Aug. 11, 2021: "Molecular Dynamics Simulations of Ferroelectric Perovskite Oxide Alloys Using Bond-Valence-Based Interatomic Potentials," *2021 Joint Nanoscience and Neutron Scattering User Meeting*, Oak Ridge, TN (virtual).
2. Jan. 27, 2021: "Electrocatalytic H_2 Evolution on Nickel Phosphides and the Role of Surface Reconstruction," *Catalysis Talks* (virtual).
1. Jul. 28, 2020: "Computational Design of Kesterite Solar Cells via Ion Substitution," *Virtual Conference on Theoretical Chemistry (VCTC)*, Stanford, CA (virtual).

C. Panels

2. Sep. 13, 2023: *International Forum on Hydrogen Production Technologies* (virtual)
1. Jul. 28, 2020: *Virtual Conference on Theoretical Chemistry (VCTC)*, Stanford, CA (virtual).

D. Contributed Talks and Posters

24. Aug. 13, 2023: "(Ca,Ce)(Ti,Mn)O_3 perovskites for two-step solar thermochemical H_2 production," talk at the *ACS Fall Meeting*, San Francisco, CA.

23. Jul. 6, 2023: "Surface Phase Diagrams from Nested Sampling," talk at *MaxEnt2023*, Garching, Germany. (presented by Ray Yang)

22. Jun. 8, 2023: "Surface Phase Diagrams from Nested Sampling," talk at the *32nd Annual Midwest Thermodynamics and Statistical Mechanics Conference*, Notre Dame, IN. (presented by Ray Yang)

21. Jun. 7, 2023: "Path of Least Resistance: Predictive Thermochemical Cycles for Bulk and Surface Catalysis," talk at the *32nd Annual Midwest Thermodynamics and Statistical Mechanics Conference*, Notre Dame, IN.

20. Mar. 29, 2023: "Extended Born-Haber cycle for explaining oxygen-chlorine chemisorption scaling on transition metals," talk at the *ACS Spring Meeting*, Indianapolis, IN.

19. Mar. 8, 2023: "Extended Born-Haber cycle for explaining oxygen-chlorine chemisorption scaling on transition metals," talk at the *APS March Meeting*, Las Vegas, NV.

18. Nov. 15, 2022: "Crystal Features Controlling Oxygen Vacancy Formation in ABO_3 Perovskites," talk at the *AIChE Annual Meeting*, Phoenix, AZ.

17. Jun. 30, 2022: "Intuitive materials design for solar thermochemical carbon dioxide splitting," talk at the *19th International Conference on Carbon Dioxide Utilization (ICCDU)*, Princeton, NJ.

16. Mar. 16, 2022: "Crystal Features Controlling Oxygen Vacancy Formation in ABO_3 Perovskites," talk at the *APS March Meeting*, Chicago, IL.

15. Apr. 6, 2021: "Efficient Machine-Learned Model for Oxide Perovskite Performance in Solar Thermochemical Technologies," talk at the *ACS Spring Meeting*, San Antonio, TX (virtual).

14. Nov. 19, 2020: "Codoping Cu_2ZnSnS_4 with Cd, Ge, and Se: a recipe for suppressing deep traps," talk at the *ACS 2020 Virtual Postdoc Symposium*, San Francisco, CA (virtual).

13. Nov. 17, 2020: "Suppressing Deep-Trap Formation in Cu_2ZnSnS_4-Based Solar Cells," talk at the *AIChE Annual Meeting*, San Francisco, CA (virtual).

12. Nov. 16, 2020: "Scratching the Surface: Simulating and Engineering the Interfaces of Materials for Sustainable Energy and Environmental Remediation," poster at the *AIChE Annual Meeting*, San Francisco, CA (virtual).

11. Nov. 16, 2020: "Transferable Bond Valence Interatomic Potentials for the Accurate and Reliable Nanoscale Simulation of Ferroelectric Solid Solutions," talk at the *AIChE Annual Meeting*, San Francisco, CA (virtual).

10. Aug. 17, 2020: "Codoping Cu2ZnSnS4 with Cd, Ge, and Se: a recipe for suppressing deep traps," talk at the *ACS Fall Meeting*, San Francisco, CA (virtual).

9. Jul. 29, 2020: "Exchange-correlation functional challenges in modeling chalcogenides," poster at the *Virtual Conference on Theoretical Chemistry (VCTC)*, Stanford, CA (virtual).

8. Mar. 25, 2020: "Codoping Cu_2ZnSnS_4 with Ge and Se: Recipe for suppressing deep traps," talk at the *ACS Spring Meeting*, Philadelphia, PA (canceled due to COVID-19).

7. Mar. 3, 2020: "Suppressing deep-trap formation in Cu_2ZnSnS_4-based solar cells," talk at the *APS March Meeting*, Denver, CO (canceled due to COVID-19).

6. Nov. 15, 2019: "Tuning HER on Nickel Phosphide Using Chemical Pressure: First Principles and Machine Learning," talk at the *AIChE Annual Meeting*, Orlando, FL.

5. Nov. 14, 2019: "Predicting the Surface Phase Diagram of Ag(111) Using Ab Initio Grand Canonical Monte Carlo," talk at the *AIChE Annual Meeting*, Orlando, FL.

4. Apr. 3, 2019: "Predicting the surface phase diagram of Ag(111) using ab initio grand canonical Monte Carlo," talk at the *ACS Spring Meeting*, Orlando, FL.

3. Mar. 5, 2019: "Predicting the surface phase diagram of Ag(111) using ab initio grand canonical Monte Carlo," talk at the *APS March Meeting*, Boston, MA.

2. Aug. 12-20, 2015: "First-principles investigation of the hydrogen evolution reaction on nickel phosphides Ni_2P and Ni_5P_4," talk at the *ACS Fall Meeting*, Boston, MA.

1. Mar. 21, 2013: "The Role of Water in Surface Charge Transport on Tin Dioxide as Revealed by the Thermal Dependence of Conductance," talk at the *APS March Meeting*, Baltimore, MD.

CURRENT EXTRAMURAL FUNDING SOURCES

2. **Department of Energy, Energy Efficiency & Renewable Energy, Hydrogen & Fuel Cell Technologies**
   Award Number: DE-EEDE-EE0010733
   Start Date: TBD
   Duration: Three years
   Award Amount: $1,000,000 (full grant D+ID), $430,000 (my allocation of D+ID)

1. **National Science Foundation, Division Of Chemistry, Macromolec/Supramolec/Nano**
   Award Number: 2305155
   Start Date: August 1, 2023
   Duration: Three years
   Award Amount: $176,693 (full grant D+ID), $176,693 (my allocation of D+ID)

CURRENT INTRAMURAL FUNDING SOURCES

1. **TRIADS Seed Grant**
   Start Date: April 18, 2023
   Duration: One-two years
   Award Amount: $26,500