

ROBERT F. BERGER

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APPOINTMENTS **ASSOCIATE PROFESSOR**
Western Washington University, Bellingham, WA
Department of Chemistry
2019–present

ASSISTANT PROFESSOR
Western Washington University, Bellingham, WA
Department of Chemistry
2013–2019

EDUCATION **POSTDOCTORAL**
Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley CA (2009–2013)
Advisor: Prof. Jeffrey Neaton
Topic: Atomic/electronic structure relationships in oxides for energy applications

GRADUATE
Cornell University, Ithaca NY (2005–2009)
Ph.D. in Chemistry, 2009
Advisors: Profs. Roald Hoffmann and Stephen Lee
Thesis: *Demystifying large unit-celled intermetallic crystals*

UNDERGRADUATE
Princeton University, Princeton NJ (2001–2005)
A.B. in Chemistry, 2005
Advisor: Prof. Robert Cava
Thesis: *Geometric magnetic frustration in oxides with triangular planar lattices*

AWARDS **FACULTY**
Peter J. Elich Excellence in Teaching Award, 2024
Cottrell Scholar Award (Research Corporation for Science Advancement), 2017

GRADUATE
Tunis Wentink Prize (Top two graduating Ph.D. students in Cornell chemistry), 2009
Howard Neal Wachter Memorial Prize (Physical chemistry), 2008
Bayer Teaching Excellence Award, 2007

UNDERGRADUATE
Magna Cum Laude, 2005
Phi Beta Kappa Society (Academic honor society), 2005
Sigma Xi Society (Scientific research society), 2005
Robert Thornton McKay Prize (Physical chemistry), 2005
William Foster Memorial Prize (Chemistry), 2004
Shapiro Prize for Academic Excellence, 2002
Manfred Pyka Memorial Prize (Physics), 2002

Western Washington University *undergraduate student, †master's student

33. Berger, RF; Amacher, JF. "Implementation of professional development initiatives in chemistry at a regional public university". *ACS Symposium Series: Professional Mentoring Programs for Science Students* (2024), eds. AR Urbach and PJ Beuning, accepted for publication.
32. Urbach, AR; Berger, RF; Beuning, PJ; Nevidomskyy, AH. "COMPASS: Career and Occupational Mentoring for the Professional Advancement of Science Students". *ACS Symposium Series: Professional Mentoring Programs for Science Students* (2024), eds. AR Urbach and PJ Beuning, accepted for publication.
31. Clover, AW[†]; Jones, AP*; Berger, RF; Kaminsky, W; O'Neil, GW. "Regioselective fluorohydrin synthesis from allylsilanes and evidence for a silicon-fluorine gauche effect". *J. Org. Chem.* (2024), in press.
30. Baiz, CR; Berger, RF; Donald, KJ; de Paula, JC; Fried, SD; Rubenstein, B; Stokes, GY; Takematsu, K; Londergan, C. "Lowering Activation Barriers to Success in Physical Chemistry (LABSIP): A community project". *J. Phys. Chem. A* (2023), *128*, 3–9.
29. Anunobi, MO*; Berger, RF. "Energetic stability and band-edge orbitals of layered inorganic perovskite compounds for solar energy applications". *J. Phys. Chem. C* (2023), *127*, 20217–20225.
28. Berger, RF. "Electronic structure of oxide and halide perovskites". In *Comprehensive Inorganic Chemistry III* (2023), eds. J Reedijk and KR Poeppelemeier, vol. 3, 4–25.
27. Teply, C[†]; Tyler, BA[†]; Berger, RF. "Tuning the band gaps of oxide and halide perovskite compounds via biaxial strain in all directions". *J. Phys. Chem. C* (2021), *125*, 25951–25958.
26. Cirlincione, DV*; Berger, RF. "Tuning the electronic structure of d^0 perovskite oxides by combining distortive modes". *Phys. Rev. B* (2021), *103*, 045127.
25. Steele, JA; Jin, H; Dovgaliuk, I; Berger, RF; Braeckevelt, T; Yuan, H; Martin, C; Solano, E; Lejaeghere, K; Rogge, SMJ; Notebaert, C; Vandezande, W; Janssen, KPF; Goderis, B; Debroye, E; Wang, Y-K; Dong, Y; Ma, D; Saidaminov, M; Tan, H; Lu, Z; Dyadkin, V; Chernyshov, D; Van Speybroeck, V; Sargent, EH; Hofkens, J; Roeyffers, MBJ. "Thermal unequilibrium of strained black CsPbI₃ thin films". *Science* (2019), *365*, 679–684.
24. McClarin, GR*; Berger, RF. "Confluence of structural distortion and A-site composition in the band gaps of perovskite niobate and tantalate photocatalysts". *Phys. Rev. B* (2019), *100*, 045202.
23. Grabill, LP[†]; Berger, RF. "Calibrating the extended Hückel method to quantitatively screen the electronic properties of materials". *Sci. Rep.* (2018), *8*, 10530.
22. Berger, RF. "Design principles for the atomic and electronic structure of perovskite photovoltaic materials: Insights from computation". *Chem. Eur. J.* (2018), *24*, 8708–8716.
21. Gormley, EL*; Berger, RF. "Binding maps for the study and prediction of bimetallic catalyst surface reactions: The case of methanol oxidation". *Int. J. Quantum Chem.* (2018), *118*, 25606.
20. Tsui, KY*; Onishi, N*; Berger, RF. "Tolerance factors revisited: Geometrically designing the ideal environment for perovskite dopants". *J. Phys. Chem. C* (2016), *120*, 23293–23298.
19. Cheung, PM*; Berger, RF; Zakharov, LN; Gilbertson, JD. "Square planar Cu(I) stabilized by a pyridinediimine ligand". *Chem. Commun.* (2016), *52*, 4156–4159.
18. Grote, C*; Berger, RF. "Strain tuning of tin-halide and lead-halide perovskites: A first-principles atomic and electronic structure study". *J. Phys. Chem. C* (2015), *119*, 22832–22837.
17. Delgado, M*; Sommer, SK*; Swanson, SP*; Berger, RF; Seda, T; Zakharov, LN; Gilbertson, JD. "Probing the protonation state and the redox-active sites of pendant base iron(II) and zinc(II) pyridinediimine complexes". *Inorg. Chem.* (2015), *54*, 7239–7248.

- Grote, C*; Ehrlich, B*; Berger, RF. “Tuning the near-gap electronic structure of tin-halide and lead-halide perovskites via changes in atomic layering”. *Phys. Rev. B* (2014), *90*, 205202.

POSTDOCTORAL

- Berger, RF; Broberg, DP; Neaton, JB. “Tuning the electronic structure of SrTiO₃/SrFeO_{3-x} superlattices via composition and vacancy control”. *APL Materials* (2014), *2*, 046101.
- Poloni, R; Lee, K; Berger, RF; Smit, B; Neaton, JB. “Understanding trends in CO₂ adsorption in metal-organic frameworks with open-metal sites”. *J. Phys. Chem. Lett.* (2014), *5*, 861–865.
- Goldstein, AP; Andrews, SC; Berger, RF; Radmilovic, VR; Neaton, JB; Yang, P. “Zigzag inversion domain boundaries in indium zinc oxide-based nanowires: Structure and formation”. *ACS Nano* (2013), *7*, 10747–10751.
- Lee, C-H; Podraza, NJ; Zhu, Y; Berger, RF; Shen, S; Sestak, M; Collins, RW; Kourkoutis, LF; Mundy, JA; Wang, H; Mao, Q; Xi, X; Brillson, LJ; Neaton, JB; Muller, DA; Schlom, DG. “Effect of reduced dimensionality on the optical band gap of SrTiO₃”. *Appl. Phys. Lett.* (2013), *102*, 122901.
- Berger, RF; Neaton, JB. “Computational design of low-band-gap double perovskites”. *Phys. Rev. B* (2012), *86*, 165211.
- Berger, RF; Fennie, CJ; Neaton, JB. “Band gap and edge engineering via ferroic distortion and anisotropic strain: The case of SrTiO₃”. *Phys. Rev. Lett.* (2011), *107*, 146804.

GRADUATE

- Berger, RF; Walters, PL; Lee, S; Hoffmann, R. “Connecting the chemical and physical viewpoints of what determines structure: From 1-D chains to γ -brasses”. *Chem. Rev.* (2011), *111*, 4522–4545.
- Berger, RF; Lee, S; Johnson, J; Nebgen, B; So, ACY. “Laves phases, γ -brass, and 2×2×2 superstructures: A new class of quasicrystal approximants and the suggestion of a new quasicrystal”. *Chem. Eur. J.* (2008), *14*, 6627–6639. (Cover)
- Berger, RF; Lee, S; Johnson, J; Nebgen, B; Sha, F; Xu, J. “The mystery of perpendicular fivefold axes and the fourth dimension in intermetallic structures”. *Chem. Eur. J.* (2008), *14*, 3908–3930.
- Berger, RF; Lee, S; Hoffmann, R. “A quantum mechanically guided view of Mg₄₄Rh₇”. *Chem. Eur. J.* (2007), *13*, 7852–7863. (Cover)

UNDERGRADUATE

- Hemmida, M; Krug von Nidda, H-A; Büttgen, N; Loidl, A; Alexander, LK; Nath, R; Mahajan, AV; Berger, RF; Cava, RJ; Singh, Y; Johnston, DC. “Vortex dynamics and frustration in two-dimensional triangular chromium lattices”. *Phys. Rev. B* (2009), *80*, 054406.
- Hsieh, D; Qian, D; Berger, RF; Cava, RJ; Lynn, JW; Huang, Q; Hasan, MZ. “Magnetic excitations in triangular lattice NaCrO₂”. *J. Phys. Chem. Solids* (2008), *69*, 3174–3175.
- Hsieh, D; Qian, D; Berger, RF; Cava, RJ; Lynn, JW; Huang, Q; Hasan, MZ. “Unconventional spin order in the triangular lattice system NaCrO₂: A neutron scattering study:”. *Physica B* (2008), *403*, 1341–1343.
- McQueen, T; Huang, Q; Lynn, JW; Berger, RF; Klimczuk, T; Ueland, BG; Schiffer, P; Cava, RJ. “Magnetic structure and properties of the S=5/2 triangular antiferromagnet α -NaFeO₂”. *Phys. Rev. B* (2007), *76*, 024420.
- Olariu, A; Mendels, P; Bert, F; Ueland, BG; Schiffer, P; Berger, RF; Cava, RJ. “Unconventional dynamics in triangular Heisenberg antiferromagnet NaCrO₂”. *Phys. Rev. Lett.* (2006), *97*, 167203.

GRANT FUNDING

- National Science Foundation, Standard Grant (lead PI Mark Bussell), 2021–2024, \$366,514

“RUI:CAS: Metal phosphides on nanostructured indium oxide – New photocatalysts for CO₂ hydrogenation”

7. National Science Foundation, Standard Grant, 2021–2023, \$268,067
“RUI: Confronting structural complexity in the computational design and understanding of perovskite materials for solar energy conversion”
6. Western Washington University AMSEC, Seed Grant (with Mark Bussell), 2020, \$6,400
“Metal phosphide-oxide catalysts for solar fuels production”
5. Western Washington University, Summer Teaching Grant, 2020, \$6,000
“Flipping the physical chemistry series to optimize student learning”
4. Research Corporation, Cottrell Scholar Award, 2017–2021, \$100,000
“Novel approaches to the computational understanding and prediction of perovskite dopant environments and distortive modes”
3. Research Corporation, Cottrell College Science Award, 2015–2017, \$55,000
“Efficient computational screening and chemical understanding of oxide nanostructures for energy applications”
2. XSEDE, Research Allocation, 2015–2016, 167,000 CPU-hours, est. \$11,209
“Design and understanding of novel methanol oxidation catalysts using site-specific binding maps”
1. Western Washington University, Project Development Award, 2015, \$8,000
“Computational design of novel methanol oxidation catalysts”

TALKS

11. Western Washington Data-Driven Discovery Seminar Series, October 2022 (Invited)
“Shining light on perovskites”
10. ACS National Meeting, August 2017, Washington, DC (Contributed)
“Tuning the band-edge orbitals of perovskite photovoltaic materials”
9. ACS National Meeting, March 2016, San Diego, CA (Invited)
“Computational design of perovskite nanostructures for solar energy conversion”
8. APS March Meeting, March 2013, Baltimore, MD (Contributed)
“Tuning the electronic structure of (SrTiO₃)_n/(SrFeO_{3-x})₁ superlattices”
7. Molecular Foundry Annual Users’ Meeting, October 2012, Berkeley, CA (Invited)
“First-principles studies of SrTiO₃ and related compounds for solar water splitting”
6. Molecular Foundry Seminar Series, September 2012, Berkeley, CA (Invited)
“First-principles studies of SrTiO₃ and double perovskites for solar water splitting”
5. APS March Meeting, March 2012, Boston, MA (Invited)
“Band gap and edge engineering of SrTiO₃ via ferroic distortion and anisotropic strain”
4. Reed College Physics Department Seminar, October 2011, Portland, OR (Invited)
“Tuning the electronic structure of SrTiO₃ for solar water splitting”
3. APS March Meeting, March 2011, Dallas, TX (Contributed)
“Optical properties of epitaxial Sr-Ti-O compounds from first principles”
2. MRS Fall Meeting, November 2010, Boston, MA (Contributed)
“Manipulating the band gap of SrTiO₃ via strain-controlled phase transitions”
1. APS March Meeting, March 2010, Portland, OR (Contributed)
“First-principles study of the electronic properties of biaxially strained SrTiO₃”

RESEARCH MENTORING

FACULTY, WESTERN WASHINGTON UNIVERSITY

- Mentored 22 undergraduate students and 5 master’s students to date
- Co-authored 18 papers with 17 WWU undergraduate and master’s students

STUDENT RESEARCH AWARDS

- Jill Addington: Outstanding Undergraduate Poster Award, ACS National Meeting 2022
- Geoffrey McClarin: Outstanding Poster Award, ACS Northwest Regional Meeting 2018
- Nicole Onishi: Outstanding Poster Award, WWU Scholars Week 2017
- Ka Yi Tsui and Nicole Onishi: Outstanding Poster Award, WWU Scholars Week 2016

- Christopher Grote: Outstanding Poster Award, WWU Scholars Week 2015
- Ryan Hackler: Outstanding Poster Award, WWU Scholars Week 2014

STUDENT POSTER PRESENTATIONS

- Kevin Sweeney, WWU Scholars Week, 2023
“Computational analysis of carbon monoxide adsorption and hydrogen dissociative adsorption on nickel phosphide surfaces”
- Zen Graham, WWU Scholars Week, 2023
“Structural stability and tunability of bandgaps in mixed tin-germanium perovskites”
- Jill Addington, ACS National Meeting and WWU Scholars Week, 2022
“Density functional theory analysis of halide double perovskites for solar energy conversion”
- Oluchi Anunobi, Murdock Conference and WWU Scholars Week, 2021 and 2022
“Rationalizing the energetic stability of layered inorganic perovskites for solar energy conversion”
- Corey Teply, ACS Northwest Regional Meeting, 2021
“Band gap engineering of perovskites via strain in all directions for solar applications”
- Jill Addington, MERCURY Conference, 2021
“Density functional theory analysis of halide perovskites for solar energy conversion”
- Geoffrey McClarin, WWU Scholars Week, 2019
“Band gap and edge engineering of perovskite niobate and tantalate photocatalysts”
- Sydney Sipes-Hayse, WWU Scholars Week, 2018
“Relating strain, distortion, and electronic properties in perovskite materials”
- Haley Doran, ACS Northwest Regional Meeting and WWU Scholars Week, 2018
“Computational design of double perovskites for photovoltaic applications”
- Geoffrey McClarin, ACS National Meeting and WWU Scholars Week, 2018
“Band gap and edge engineering of perovskite niobate and tantalate photocatalysts”
- Joshua Welsh, WWU Scholars Week, 2017
“Computational understanding and tuning of exotic distortions in perovskite materials”
- Geoffrey McClarin, WWU Scholars Week, 2017
“Computational identification of novel antiferroelectric perovskite materials”
- Nicole Onishi, Theory and Applications of Computational Chemistry Conference, 2016
“Geometrically designing the ideal environment for perovskite dopants”
- Linda Grabill, WWU Scholars Week, 2016
“Toward accurate and efficient computational screening of the electronic structure and band gaps of semiconductors”
- Adam Elder, WWU Scholars Week, 2016
“Computational screening of crystalline surfaces for interface stability”
- Ka Yi Tsui and Nicole Onishi, Dreyfus Poster Session and WWU Scholars Week, 2016
“Geometrically designing the ideal environment for perovskite dopants”
- Linda Grabill, WWU Scholars Week, 2015
“Toward accurate and efficient band structure calculations of solar energy conversion materials”
- Eoghan Gormley, WWU Scholars Week, 2015
“A computational approach to methanol oxidation catalyst design”
- Christopher Grote, MRS National Meeting and WWU Scholars Week, 2015
“Tuning the electronic structure of tin and lead halide perovskites through layering, strain, and distortion”
- Bradley Ehrlich and Christopher Grote, WWU Scholars Week, 2014
“Tuning the electronic structure of lead halide and tin halide perovskites for solar energy conversion via changes in atomic layering”
- Christopher Grote, Pauling Symposium, 2014
“The effects of atomic layering, strain, and distortions on the band gaps of tin and lead halide perovskites”

1. Ryan Hackler, ACS Undergraduate Symposium, 2014
“Theoretical investigations on bimetallic nanoparticle activity for methanol oxidation”

TEACHING**FACULTY, WESTERN WASHINGTON UNIVERSITY**

- CHEM 121/161, General Chemistry I (lecture 3 times, lab 1 time)
- CHEM 125, Honors General Chemistry I (2 times)
- CHEM 401, Independent Research in Chemistry (4 times)
- CHEM 461, Physical Chemistry I (Quantum Mechanics) (6 times)
- CHEM 462, Physical Chemistry II (Stat. Mech. and Thermodynamics) (8 times)
- CHEM 463, Physical Chemistry III (Equilibrium and Kinetics) (5 times)
- CHEM 464, Physical/Inorganic Chemistry Lab I (8 times)
- CHEM 465, Physical/Inorganic Chemistry Lab II (9 times)
- CHEM 486/586, Computational Chemistry (co-taught with Tim Kowalczyk) (4 times)
- CHEM 497L/597L, Solid State Chemistry (1 time)
- CHEM 596, Seminar in Chemistry and Biochemistry (3 times)

**PROFESSIONAL
DEVELOPMENT****WWU COLLEGE OF SCIENCE & ENGINEERING**

- Participating in BETTER in STEM workshops, 2022–present
- Participated in Advancing Excellence and Equity in Science (AEES) workshops, 2017–2019
- Participated in ISMs (equity and inclusion) workshops, 2017

SERVICE**WWU DEPARTMENT OF CHEMISTRY**

- General chemistry coordination team (committee chair), 2021–present
- Department meeting scribe, 2023–2024
- Policies and procedures taskforce, 2021–2023
- Search committees: Chemistry education tenure-track faculty, 2022 (committee chair); General chemistry laboratory coordinator, 2021; Chemistry education tenure-track faculty, 2019; Analytical chemistry non-tenure-track faculty, 2015; Instrument specialist, 2015; Computational materials tenure-track faculty (joint with AMSEC), 2014
- Seminar coordinator, fall 2021, fall 2015, winter 2015
- Assessment committee (committee chair), 2018–2020
- Department newsletter, 2017–2023
- Western Preview, 2017
- General chemistry taskforce, 2016–2018
- Curriculum and/or enrollment committee, 2016–present
- Advisor to chemistry and biochemistry majors, 2014–present
- Graduate committee, 2014–2016
- Web/technology committee, 2013–2016
- Library liaison, 2013–2020

WWU ADVANCED MATERIALS SCIENCE & ENGINEERING CENTER (AMSEC)

- Scholarship and fundraising committee, 2017–2018 and 2021–present
- Search committee: Computational materials tenure-track faculty, 2014
- Compass 2 Campus energy demonstrations, 2014–2017

WWU COLLEGE OF SCIENCE & ENGINEERING

- Mentor in Advancing Excellence and Equity in Science (AEES) program, 2019–2023
- Technical operations committee, 2015–2020

WESTERN WASHINGTON UNIVERSITY

- Academic technology committee, 2022–present

ACADEMIC COMMUNITY

- Co-founder and co-organizer of LABSIP (Lowering Activation Barriers to Success in P-Chem), 2022–present
- Executive committee of MERCURY (Molecular Education and Research Consortium in Undergraduate Computational Chemistry), 2020–present
- Co-founder and co-organizer of COMPASS workshops (Career and Occupational Mentoring for the Professional Advancement of Science Students), 2017–2023
- ACS NORM (Northwest Regional Meeting) physical chemistry session chair, 2021
- National Science Foundation grant panel reviewer, 2021 and 2023
- Ad hoc reviewer for: National Science Foundation, US Department of Energy, Research Corporation for Science Advancement, ACS Petroleum Research Fund, and a variety of chemistry and physics journals