

Wennie Wang

wwwennie@che.utexas.edu | wangmaterialsgroup.com | github.com/wangmatgroup

University of Texas at Austin

Assistant Professor, McKetta Department of Chemical Engineering

Austin, TX
2022-current

University of Chicago, Pritzker School of Molecular Engineering (PME)

Postdoctoral Scholar, Adviser: Giulia Galli

Chicago, IL
2018-2021

University of California, Santa Barbara (UCSB), Materials Department

Ph.D. in Computational Materials, Adviser: Chris G. Van de Walle

Thesis: The Influence of High Doping on Electronic and Optical Properties of WO_3

Santa Barbara, CA
Spring 2018

Massachusetts Institute of Technology (MIT)

B.S. in Materials Science and Engineering

Thesis: Towards structural health monitoring in carbon nanotube reinforced composites

Cambridge, MA
June 2013

Areas of Interest

- First-principles methods and calculations for optoelectronic properties in semiconductors in energy- and environmentally-oriented applications
- Science policy, education outreach, diversity and inclusion efforts and strategies

Publications

*= equal contribution; ^ = undergraduate researcher, #= corresponding author

In Preparation

- J.-L. Ng, **W. Wang**[#]. “Assessment of density functional theory methods on bulk and electronic properties of β -NiOOH Structural Models.”
- A.M. Anderson[^], **W. Wang**[#]. “First-principles investigation of iron oxyhydroxides as electrocatalysts.”
- B.H. Lee, **W. Wang**[#]. “Physics-informed trends in adsorption of impurities on monolayer transition metal dichalcogenides.”
- E. Murhula, **W. Wang**, C. Gibson. “Crystal Structure and Surface Stability of Montebasite and Spodumene from First Principles: Implications for Lithium Extraction.”

Peer-reviewed Publications

- G. Melani, **W. Wang**, F. Gygi, K.-S. Choi, G. Galli. “Effects of solvation and temperature on the energetics of BiVO_4 surfaces with varying composition for solar water splitting.” 2024. Under Review. [arXiv].
- R. Anvari, **W. Wang**[#]. “Nature of point defects in monolayer MoS_2 and the $\text{MoS}_2/(111)\text{-Au}$ heterojunction.” *J. Appl. Phys.* 135, 174304 (2024). *Defects in Semiconductors 2024* special edition. [doi: 10.1063/5.0205981] [arXiv]
- **W. Wang**^{*}, M. Favaro^{*}, E. Chen[^], L. Trotochaud, H. Bluhm, K.-S. Choi, R. van de Krol, D.E. Starr, G. Galli. “Influence of excess charge on water adsorption on the $\text{BiVO}_4(010)$ surface.” *J. Am. Chem. Soc.*, 144, 37, 17173–17185 (2022) [doi : 10.1021/jacs.2c07501].
- (invited) **W. Wang**, A. Radmilovic, K.-S. Choi, G. Galli. “Investigating photoelectrodes for solar water splitting at the microscopic scale” *Acc. Chem. Res.* 54, 3863–3872 (2021) [doi:10.1021/acs.accounts.1c00418]
- H. Vo^{*}, S. Zhang^{*}, **W. Wang**^{*}, G. Galli, “Lessons learned from first-principles calculations of transition metal oxides.” *J. Chem. Physics.* (2021) Special Collection: in honor of Women in Chemical Physics and Physical Chemistry. 154, 174704 (2021) [doi:10.1063/5.0050353]

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- D. Lee, * **W. Wang***, C. Zhou *, X. Tong, M. Liu, G. Galli, K.-S. Choi. “The impact of surface composition on the interfacial energetics and photoelectrochemical properties of BiVO₄.” *Nature Energy*. 6, 287 (2021) [doi: 10.1038/s41560-021-00777-x] [UChicago News release][BNL news release]
- A. Lindberg*, **W. Wang***, S. Zhang, G. Galli, K.-S. Choi. “Can a PbCrO₄ photoanode perform as well as isoelectronic BiVO₄?” *ACS Appl. Energy Mater.* (2020) [doi: 10.1021/acsaem.0c01250]
- H. Ma, **W. Wang**, S. Kim, M.H. Cheng, M. Govoni, G. Galli. “PyCDFT: a Python package for constrained density functional theory.” *J. Comp. Chem.* 41, 1859 (2020) [doi: 10.1002/JCC.26354] [[open-source code](#)]
- **W. Wang**, P. Strohbeen, D. Lee, C. Zhou, J. Kawasaki, K.-S. Choi, M. Liu, G. Galli. “The role of surface oxygen vacancies in BiVO₄.” *Chemistry of Materials*. 32, 2899-2909 (2020). [doi: 10.1021/acs.chemmater.9b05047]
- **W. Wang**, Y. Kang, H. Peelaers, K. Krishnaswamy, C.G. Van de Walle. “First-principles study of transport in WO₃.” *Phys. Rev. B*. **101**, 045116 (2020). [doi: 10.1103/PhysRevB.101.045116]
- X. Zhang, J.X. Shen, **W. Wang**, C.G. Van de Walle. “First-principles Analysis of Radiative Recombination in Lead-Halide Perovskites.” *ACS Energy Letters*. 3, 2329-2334 (2018). [doi: 10.1021/acsenerylett.8b01297]
- **W. Wang**[#], H. Peelaers, J.X. Shen, C.G. Van de Walle. “Carrier-induced absorption as a mechanism for electrochromism in WO₃.” *MRS Communications*. **8**, 926-931 (2018), [doi:10.1557/mrc.2018.115]
- **W. Wang**, H. Peelaers, J.X. Shen, A. Janotti, C.G. Van de Walle. “Impact of point defects on electrochromism in WO₃.” Proc. SPIE 10533, Oxide-based Materials and Devices IX; 10533C (2018), [doi:10.1117/12.2303688]
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Phase transformations upon doping in WO₃.” *J. Chem. Phys.*, 146, 214504 (2017), [doi: 10.1063/1.4984581]
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Role of oxygen vacancies in crystalline WO₃.” *J. Mat Chem. C*, 4, 6641 – 6648 (2016), [doi: 10.1039/C6TC01643J]
- F. Kaule, **W. Wang**, S. Schoenfelder. “Modeling and Testing the Mechanical Strength of Solar Cells.” *Solar Energy Materials and Solar Cells*. 120A, 441-447 (2014) [doi: 10.1016/j.solmat.2013.06.048]
- S.S. Wicks, **W. Wang**, M.R. Williams, B.L. Wardle. “Multi-scale interlaminar fracture mechanisms in woven composite laminates reinforced with aligned carbon nanotubes.” *Composites Science and Technology*. 100, 128-135 (2014). [doi: 10.1016/j.compscitech.2014.06.003]

Patents

- Inventors: **W. Wang**, M. Hoesle M. Lang
German Patent: 2011E22406 DE/ 201206715. “*Actives Radialmagnetlager mit Polen aus hochpermabalen Material (Kobalt-Eisung Legierung)*”/” *Active Radial Magnetic Bearings with Highly Permeable Stator Material (Cobalt-Iron Alloy)*”

Honors

Fellowships

- Excellence in Research Fellowship, UCSB Institute for Energy Efficiency 2017 – 2018
- NSF Graduate Research Fellow 2014 – 2018
- Holbrook Foundation Fellowship, UCSB Institute for Energy Efficiency 2013 – 2014

Awards

- APS 5 Sigma Physicist Award (science policy) 2024
- ACS PRF Doctoral New Investigator 2024

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- UT Schechter–Wissler–Stice Teaching Excellence Award in Chemical Engineering (TEAChE) 2023
- Maria Lastra Postdoctoral Scholar Excellence Mentoring award, honorable mention PME 2020
- APS 2018 March Meeting Ken Hass Outstanding Student Paper Award Runner-up Winter 2018
- SPIE MKS Instruments Research Excellence Travel Award Winter 2018
- MRS Fall 2017 Graduate Student Award finalist (Silver Award) Fall 2017

Technical Talks/Workshops

Invited

- R. Anvari, B.H. Lee, **W. Wang**. “Towards defect engineering in memristors based on low-dimensional materials”. NanoKorea 2024. Goyang, South Korea. July 3-5, 2024.
- **W. Wang**. “Harnessing materials imperfections: case studies of ‘defects’ in materials for energy sustainability.” MRS Spring Meeting and Exhibition. April 22-26, 2024. Seattle, Washington.
- **W. Wang**. “Point defects in low-dimensional materials for next-generation memory devices.” Quantum Matters in Materials Science Workshop. NIST. Feb 21-22, 2024.
- **W. Wang**. “Computationally driven engineering of material defects for electrochemical technologies.” Center for Electrochemistry. The University of Texas at Austin. Nov 3, 2023.
- **W. Wang**. “Lessons learned on finding representative structural models in (photo)electrochemical systems” Computational Materials Chemistry Telluride Workshop. Telluride, CO. July 17-21, 2023.
- **W. Wang**. “Bridging first-principles calculations with experiment: Insights from case studies on (photo)electrochemical systems.” 152nd TMS Meeting and Exhibition. 22 March 2023. San Diego, CA
- **W. Wang**. “Embracing Imperfections: Understanding and leveraging how defects can tune the optoelectronic properties of transition metal oxides.” Stony Brook University, Condensed Matter Seminar Series. 16 April 2021.
- **W. Wang**, G. Galli. “Materials for Heterogeneous Catalysis: The interface is *still* the device.” MRS Spring Meeting and Exhibition. 22 April 2021.
- **W. Wang**. “Tuning the optical properties of complex oxides for energy applications.” *APS March Meeting*. March 5-9, 2018. Los Angeles, CA.
- **W. Wang**, H. Peelaers, J.-X. Shen, C.G. Van de Walle. “Mechanisms of electrochromism in WO₃.” *SPIE-Photonics West: Oxide-based Materials and Devices International Conference IX*. Jan 27-Feb 1, 2018. San Francisco, CA.

Contributed:

- K. Kawashima, J.-L. Ng, Y.-J. Soon, A.E.F. Milton, J.S. Archer, R.R. Vaidyula, J. Resasco, **W. Wang**, C. Buddie Mullins. “Comparing Alkaline Water Oxidation activity of Ni(OH)₂ and Ni(OH)₂ Electrocatalysts.” ECS PRiME. Oct 6-11, 2024. Honolulu, HI.
- J.-L. Ng, K. Kawashima, Y.-J. Son, J. Resasco, C.B. Mullins, **W. Wang**. “Integrated computational and experimental study of Nickel Oxyhydroxides for water splitting.” UT Austin Energy Institute Energy Week. March 26, 2024.
- J.-L. Ng, A. Anderson, **W. Wang**. “Towards structure and catalytic activity relationships of disordered transition metal (oxy)hydroxides as electrocatalysts.” 2024 ACS Spring Meeting. New Orleans, LA. March 17-21, 2024.
- **W. Wang**. “Computational insights of defects in layered materials for energy sustainability technologies.” 2024 APS March Meeting. March 3-8, 2024. Minneapolis, MN.
- R. Anvari, **W. Wang**. “Role of sulfur vacancy in the switching mechanism of MoS₂-based memristors.” 2024 APS March Meeting. March 3-8, 2024. Minneapolis, MN.
- A.M. Anderson, **W. Wang**. “Investigation of FeOOH for Mechanisms in Water-Splitting Reactions.” 2023 MRS Fall Meeting and Exhibit. EN07: Emerging Electrocatalytic Materials and Devices for Clean Energy and Environmental Applications.
- J.-L. Ng, K. Kawashima, Y.-J. Son, J. Resasco, C.B. Mullins, **W. Wang**. “Computational Modeling of Nickel Oxyhydroxides for water splitting.” UT Austin Energy Institute Energy Week. March 28, 2023.
- G. Melani, **W. Wang**, C. Zhou, M. Liu, K.-S. Choi, G. Galli. “Structure and reactivity of bismuth vanadate-water interfaces.” APS March Meeting. 9 March 2023.

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- **W. Wang**, A. Hilbrands, C. Zhou, E. Chen, M. Favaro, D.E. Starr, K.-S. Choi, M. Liu, G. Galli. “Computational and Experimental Insights into the BiVO₄(010) surface & interface for water-splitting applications.” APS March Meeting. 17 March 2022.
- **W. Wang**, A. Hilbrands, C. Zhou, E. Chen, M. Favaro, D.E. Starr, K.-S. Choi, M. Liu, G. Galli. “A tale of two surface terminations: Microscopic insights into the interaction of BiVO₄ with water in photoelectrochemical applications.” MRS Fall Meeting and Exhibition. 30 November 2021.
- **W. Wang**, D. Lee, C. Zhou, X. Tong, E. Chen, M. Favaro, D. Starr, K.S. Choi, M. Liu, G. Galli. “Tuning the surface energetics of the BiVO₄ (010) surface: A joint computational and experimental study.” APS March Meeting. March 15-19, 2021. Virtual.
- **W. Wang**. “Embracing Imperfections: Understanding and leveraging how defects can tune the optoelectronic properties of transition metal oxides.” University of Texas, Austin; Department of Chemical Engineering. 26 February April 2021.
- **W. Wang**. “Embracing Imperfections: Understanding and leveraging how defects can tune the optoelectronic properties of transition metal oxides.” New York University, Departments of Chemistry and Physics. 10 February 2021.
- **W. Wang**. “Embracing Imperfections: Understanding and leveraging how defects can tune the optoelectronic properties of transition metal oxides.” University of Utah, Department of Chemistry. 01 February 2021.
- **W. Wang**. “Embracing Imperfections: Understanding and leveraging how defects can tune the optoelectronic properties of transition metal oxides.” University of North Texas; Department of Chemistry. 25 January 2021.
- (canceled due to COVID-19) **W. Wang**, P. Strohbeen, D. Lee, C. Zhou, J. Kawasaki, K.S. Choi, M. Liu, G. Galli. “Comparing processing and growth methods for the BiVO₄ (010) surface: A joint first-principles and experimental effort.” APS March Meeting. March 2-6, 2020. Denver, CO.
- **W. Wang**, G. Galli, “Role of surface oxygen vacancies in BiVO₄.” MRS Fall Meeting. December 1-6, 2019. Boston, MA.
- **W. Wang**, M. Liu, K.S. Choi, G. Galli, “Influence of defects on surface morphology and electronic structure in BiVO₄.” APS March Meeting. March 4-8, 2019. Boston, MA.
- **W. Wang**, Y. Kang, K. Krishnaswamy, C.G. Van de Walle. “Influence of spin-orbit coupling in transport of WO₃.” *APS March Meeting*. March 5-9, 2018. Los Angeles, CA.
- **W. Wang**, H. Peelaers, J.-X. Shen, C.G. Van de Walle. “Influence of Structural Distortions on Optical Absorption in WO₃.” *MRS Fall Meeting*. November 26 – December 2, 2017. Boston, MA.
- **W. Wang**, Y. Kang, K. Krishnaswamy, B. Himmetoglu, C.G. Van de Walle. “Electron-phonon interactions in transport properties of WO₃.” *APS March Meeting*. March 13-18, 2017. New Orleans, LA.
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Electron-phonon interactions in transport properties of WO₃.” *APS March Meeting*. March 13-18, 2017. New Orleans, LA.
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Phase Transformations upon doping in WO₃.” *MSE Congress*. Sept 27-29, 2016. Darmstadt, Germany
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Phase Transformations upon doping in WO₃.” *APS March Meeting*. March 13-18, 2016. Baltimore, MD.
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Impact of oxygen vacancies on electrochromic behavior in WO₃.” *145th TMS Annual Meeting & Exhibition*. Nashville, TN. February 14-18, 2016.
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Insights into the oxygen vacancy in WO₃.” *28th ICDS*. Espoo, Finland. July 27-31, 2015.
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Uncovering the connection between dopants and defects in WO₃.” *MRS Spring Meeting*. San Francisco, CA. April 6-10, 2015.
- **W. Wang**, A. Janotti, C.G. Van de Walle. “Understanding the Oxygen Vacancy in WO₃.” *APS March Meeting*, San Antonio, TX. March 2-6, 2015. (Session S9)

Outreach Seminars

- APS 2023 March Meeting, APS FECS chair-elect and session organizer: 31.00.00 “The Early Career Scientist Experience in Times of Crises and Struggle,” 31.02.00 “What Do Early Career Physicists Do?,” 30.00.00 “International Perspective for Young Physicists from Particle to Materials”

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- **W. Wang.** “Getting to and coming from a PhD: A Perspective from Academia.” AICHE Southwest Student Regional Conference. Austin, TX. April 30, 2022.
- **W. Wang.** “Navigating the Job Market as a Physics or STEM Degree Holder (in the Era of COVID).” As APS Career Mentors Fellow; hosted by Fermilab Student and Postdoc Association. January 26, 2022.
- Panelist on “UCSB GS³: Life after PhD Career Panel.” 10 December 2021
- Panelist on “Learn from the Early Career Faculty Webinar Series- Part 1: The Application Process.” 27 July 2021, MRS OnDemand Webinar Series [link]
- **W. Wang,** G. Galli. “A fossil-free future: Water splitting and solar fuels @ PME.” UChicago Pritzker Institute of Molecular Engineering Earth Day. 21 April 2021.
- **W. Wang.** “Navigating the Job Market as a Physics or STEM Degree Holder (in the Era of COVID).” As APS Career Mentors Fellow; hosted by Prof. Lance Cooper at UIUC. December 4, 2020. [link]
- (invited) **W. Wang.** “MISTI-Germany: A student's perspective on international internships.” MSE Congress. Darmstadt, Germany. 27-29 September 2016
- N.M. Larson, **W. Wang,** D. Hwang. “Transforming the Diversity Landscape.” Symposium co-organizer and moderator. 145th TMS Annual Meeting & Exhibition. Nashville, TN. February 14-18, 2016.
- (invited) N.M. Larson, **W. Wang,** D. Hwang. “Highlights from the Transforming the Diversity Landscape Symposium: The Importance of Empathy on the Individual and Program Level.” TMS DMMM2, July 25-26, 2016. Northwestern University, Evanston, IL.

Teaching Experience

University of Texas at Austin CHE 350: Chemical Engineering Materials

Austin, TX

Instructor

Spring 2022-Spring 2024

- Undergraduate course, introduction of concepts of materials science and engineering.

University of Texas at Austin CHE 384T: Computational Methods in Materials Science

Austin, TX

Instructor

Fall 2024

- Graduate course, introduction to methods in computational methods for materials science and engineering

University of Chicago Materials Research Science and Engineering Center

Chicago, IL

Lead instructor [link]

Fall 2018-Fall 2021

UCSB MAT 188: Materials in Energy Technologies

Santa Barbara, CA

Co-Instructor

Fall 2015

- Created, organized and taught undergraduate course in collaboration with other graduate students
- [course description] [course summary]

UCSB Materials Graduate courses

Santa Barbara, CA

Teaching Assistant

Spring 2017

- MAT 228 Computational Materials (Spring 2017), MAT 211A&B Engineering Quantum Mechanics (Winter 2017, Spring 2016), MAT 200B Electronic and Atomic Structure of Materials (Winter 2015)

MIT 3.091 Introduction to Solid State Chemistry

Cambridge, MA

Teaching Assistant

Fall 2012

- Student evaluations: 6.3 out of 7

Service Experience

Journal Reviews: *Nature Energy, ACS Energy Letters, J. Am. Chem. Soc., Phys. Rev Letters, Appl. Phys. Lett., J. Chem. Phys. Lett., Phys. Rev. Mater. J. Appl. Phys., Phys. Status Solidi B, Chem. Mater., ACS Catalysis, J. Chem. Theory. Comp., J. Mater. Chem. C, New J. Chem., Phys. Rev X, Phys. Rev. X Energy, Phys. Rev. Materials, Chem. Phys., J. Am. Ceramic Soc.,*

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Grants Reviews: DOE RENEW (2022), NSF GRFP (2023, 2024), AI4Materials Design Workshop (2023), NSF CBET Catalysis (2023, 2024), DOD NSDEG (2024), ACS PRF (2024)

Department Service: OXE Faculty advisor (Spring 2023-); Junior Faculty mentor (2023-); Faculty Search (2023), Graduate Admissions Committee (2022, 2023); ChE Best Paper Committee (2024)

University Service: AI faculty cluster hire (2024),

Workshops: “Systematic Analysis of Errors and Uncertainty Across Scales from Materials Modeling & Discovery to Manufacturing: Towards Best Practices.” Basic Research Innovation Collaboration Center (BRICC) on June 8-9, 2023 in Arlington, VA. Discussion leader.

Conferences: AIChE Area 8, session co-chair, “Characterization, Theory, and Data Science for Electronic and Photonic Materials” (Fall 2024)

APS Forum for Early Career Scientists (FECS)

- Member-at-large (2020-2021): FECS member COVID survey, March Meeting Travel Grant,
- Chair-line (2021-2024): March Meeting Travel Grant (2021-2024), initiation of APS–EPS–ICTP international award for early-career researchers (2023), March Meeting Poster competition (2022, 2023, 2024), initiation of national standard for graduate student pay, support for APS 2023 Wiki Scientist Course, APS FECS Diversity and Inclusion Award (2022, 2023), collaboration with APS Government Affairs on Keep STEM Talent Act (2023)

APS Career Mentoring Fellow

2020-current

UCSB Beyond Academia Annual Career Conference (<https://beyondacademiaucsb.org/>)

2015-2018

- Co-founder, executive Committee organizer and panel moderator
- Interfaced with university and industry officials to raise and oversee \$25,000 funds for organizing annual conference with > 150 attending graduate students and postdocs

UCSB Graduate Students for Diversity in Science (<http://gsds.mrl.ucsb.edu/>)

2014-2018

- President (2016-2017), Outreach Director (2015-2016)
- Oversaw and coordinated group of 30-40 graduate students for inviting speakers, outreach to local college campuses, and on-campus partnerships quarterly

UCSB Science Line

Spring 2014-Spring

2018

- Certificate of Excellence for answering 2015, 2016