

Wennie Wang

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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

Santa Barbara, CA
Spring 2018

Massachusetts Institute of Technology (MIT)

B.S. in Materials Science and Engineering

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

- (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]
- 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/acsenergylett.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]

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- **W. Wang**, H. Peelaers, J.X. Shen, A. Janotti, C.G. Van de Walle. “Impact of point defects on electrochromism in WO_3 .” 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 WO_3 .” *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 WO_3 .” *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 hochpermeabalen Material (Kobalt-Eisung Legierung)*”/” *Active Radial Magnetic Bearings with Highly Permeable Stator Material (Cobalt-Iron Alloy)*”

Teaching Experience

University of Texas at Austin

Instructor

Austin, TX

Spring 2022

- CHE 350: Chemical Engineering Materials. Undergraduate course, introduction of concepts of materials science and engineering.

University of Chicago Materials Research Science and Engineering Center

Lead instructor [link]

Chicago, IL

Fall 2018-Fall 2021

UCSB MAT 188: Materials in Energy Technologies

Co-Instructor

Santa Barbara, CA

Fall 2015

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

UCSB Materials Graduate courses

Teaching Assistant

Santa Barbara, CA

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)

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

- Maria Lastra Postdoctoral Scholar Excellence Mentoring award, PME
 - Fall 2019 (nominated), Fall 2020 (honorable mention)
- APS 2018 March Meeting Ken Hass Outstanding Student Paper Award Runner-up Winter 2018

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- SPIE MKS Instruments Research Excellence Travel Award Winter 2018
- MRS Fall 2017 Graduate Student Award finalist (Silver Award) Fall 2017

Technical Talks

- **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**, G. Galli “Materials for Heterogeneous Catalysis: The interface is *still* the device.” MRS Spring Meeting and Exhibition. 22 April 2021.
- (invited) **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**, 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.
- (Invited) **W. Wang**. “Tuning the optical properties of complex oxides for energy applications.” *APS March Meeting*. March 5-9, 2018. Los Angeles, CA.
- **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.
- (Invited) **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.
- **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.

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- **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 Efforts

- **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.
- 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.

Service Experience

Reviewer: *Nature Energy, J. Am. Chem. Soc., Chem. Mater., ACS Catalysis, J. Chem. Phys. Lett., Phys. Rev. Mater. J. Appl. Phys., Phys. Status Solidi B, J. Chem. Theory. Comp., J. Mater. Chem. C, New J. Chem.*

APS Forum for Early Career Scientists

- Member-at-large (2020-2021)
- Chair (2021-2024)

APS Career Mentoring Fellow

2020, 2021, 2022

"Navigating the Job Market as a Physics or STEM Degree Holder (in the Era of COVID)"; Fall 2020 Virtual Physics Careers Seminar Series, 4 Dec. 2020, hosted by Prof. Lance Cooper

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