# Wennie Wang

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## Education

University of Chicago, Pritzker School of Molecular Engineering (PME) — Chicago, IL
*Postdoctoral Scholar* — Summer 2018-current

University of California, Santa Barbara (UCSB): — Santa Barbara, CA
*Ph.D. in Computational Materials* — Spring 2018
- NSF Graduate Research Fellow — 2014 –2018
- Excellence in Research Fellows, UCSB Institute for Energy Efficiency — 2017 –2018
- Holbrook Foundation Fellow, UCSB Institute for Energy Efficiency — 2013 –2014

Massachusetts Institute of Technology (MIT): — Cambridge, MA
*B.S. in Materials Science and Engineering* — June 2013

## Research Interests

- First-principles computational methods of transition metal extended systems to discover microscopic understanding of optical, electronic, and transport properties in energy sustainability technologies

## Research Experience

**University of Chicago, Pritzker School of Molecular Engineering (PME)** — Chicago, IL
*Postdoctoral Scholar, Adviser: Giulia Galli* — Summer 2018 - current
- Density functional theory, molecular dynamics simulations, and many-body perturbation theory on complex oxide surfaces and interfaces for water-splitting technologies
- Collaborated with experimentalists from University of Wisconsin-Madison, Brookhaven National Lab, Helmholtz Zentrum Berlin
- Resulted in 3 conferences (1 pending), 4 papers (including 3 first author/equal contribution).

**UCSB Materials Department** — Santa Barbara, CA
*Graduate Student Researcher, Adviser: Chris G. Van de Walle* — Fall 2013 – Spring 2018
- Ab-initio calculations for defects and impurities in oxides for energy efficiency applications
- Elucidating mechanisms of electrochromism, transport, phase transformations in transition metal oxides
- Communicated results in 12 conferences (including 2 invited), 6 publications (including 5 first author)
- Thesis: "The Influence of High Doping on Electronic and Optical Properties in Tungsten Oxide" [link]

**MIT NECST Lab** — Cambridge, MA
*Student researcher, Undergraduate Research Opportunities Program (UROP)* — Fall 2011- Spring 2013
- Mechanical testing of carbon nanotube fiber reinforced composites for structural health monitoring
- Collaborated with Metis, Corp resulting in 1 paper and undergraduate thesis
- Thesis: "Towards structural health monitoring in carbon nanotube reinforced composites" [link]

**Fraunhofer Institute CSP** — Halle (Saale), Germany
*Student Intern, Adviser: Stefan Schoenfelder* — Summer 2012
- Modeled mechanical properties and fracture mechanics of solar cell metallization systems
- Resulted in top 10 paper submission to SiliconPV 2013 conference

**Siemens AG** — Berlin, Germany
*Student intern, Adviser: Matthias Lang* — Summer 2011
- Designed /optimized stator of radial magnetic bearings using finite element and genetic algorithm
- Resulted in company-wide presentation and 1 patent (filed in Germany and U.S.)

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## Publications

* = equal contribution

- (invited review) **W. Wang**,* A. Hilbrands,* C. Zhou,* E. Chen,* M. Liu, K.-S. Choi, G. Galli. "Integrated experimental and theoretical strategies to investigate oxide surfaces and interfaces in photoelectrodes" *J. Mater. Chem. A* (2021) Under preparation.

- D. Lee,* **W. Wang***, C, Zhou *, X. Tong, M. Liu, G. Galli, K.-S. Choi. "Modifying interfacial energetics in $BiVO_4$ photoanodes by surface termination." (2020) At *Nature Energy* undergoing minor revisions.

- A. Lindberg*, **W. Wang***, S. Zhang, G. Galli, K.-S. Choi. "Can a $PbCrO_4$ photoanode perform as well as isoelectronic $BiVO_4$?" *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 $BiVO_4$." *Chem. Mater.* 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 $WO_3$." *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 $WO_3$*." 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 $WO_3$." 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]

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## Patents

- Inventors: W. Wang, 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)*"
  as of March 2015, Siemens AG is pursuing a modified version for the US patent (#2012P06715WOUS01);
  Inventors: W. Wang, M. Hoesle, M. Lang

## Awards

- (nominated) Maria Lastra Postdoctoral Scholar Excellence Mentoring award, PME — Fall 2019
- 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
- (nominated) UCSB GSA Excellence in Teaching Award — Spring 2016
- APS Ovshinsky Travel Award Honorable Mention — Winter 2016
- UCSB MRL Travel Grant — Winter 2018, Fall 2017, Winter 2017, Summer 2016, Summer 2015
- UCSB MRL Travel Fellowship to DMMM1 Conference on diversity — Summer 2014
- National Forensics League 4-time national qualifier, International Extemporaneous Speaking — Summer 2009
- National Forensics League Top 15 nationally ranked speaker — Summer 2008-2009

## Teaching Experience

**University of Chicago Materials Research Science and Engineering Center** — Chicago, IL
*Co-instructor* — Fall 2018- current

- Modern Materials Technologies, colloquium at Lindbloom High School in Chicago Public School, which enrolls predominantly students from underserved populations
- Head lectures, in-class discussions, and demonstrations/labs; mentor in pedagogy for graduate student instructors; https://mrsec.uchicago.edu/education/neighborhood/modern-materials-technology/

**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 website for syllabus: http://www.mrl.ucsb.edu/~vandewalle/mat188_2015/index.htm

**UCSB MAT 228 Computational Materials** — Spring 2017
**UCSB MAT 211 Engineering Quantum Mechanics series** — Spring 2016, Winter 2017
**UCSB MAT 200B Electronic and Atomic Structure of Materials** — Winter 2015
*Teaching Assistant*

- Graduate level courses with Profs. Chris Van de Walle and Michael Chabinyc

**MIT 3.091 Introduction to Solid State Chemistry** — Cambridge, MA
*Recitation leader* — Fall 2012

- introductory undergraduate course; received one of highest teacher evaluations (6.3 out of 7)

**Wichita State University Department of Physics** — Wichita, KS
*Assistant Researcher; Adviser: Elizabeth Behrman* — Summer 2010

- Simulated quantum neural networks capable of generalization for the factorization of large numbers
- Built demonstrations for honors Mechanics class, e.g., giant Newton's cradle out of bowling balls

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## Technical Conferences

- (submitted) **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 $BiVO_4$ (010) surface: A joint computational and experimental study." APS March Meeting. March 15-19, 2021. Virtual.

- **W. Wang**, P. Strohbeen, D. Lee, C. Zhou, J. Kawasaki, K.S. Choi, M. Liu, G. Galli. "Comparing processing and growth methods for the $BiVO_4$ (010) surface: A joint first-principles and experimental effort." APS March Meeting. March 2-6, 2020. Denver, CO. (Canceled due to COVID)

- **W. Wang,** G.Galli, "Role of surface oxygen vacancies in $BiVO_4$." 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 Angles, CA.

- **W. Wang**, Y. Kang, K. Krishnaswamy, C.G. Van de Walle. "Influence of spin-orbit coupling in transport of $WO_3$." *APS March Meeting*. March 5-9, 2018. Los Angles, CA.

- (Invited) **W. Wang**, H. Peelaers, J.-X. Shen, C.G. Van de Walle. "Mechanisms of electrochromism in $WO_3$." *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 $WO_3$." *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 $WO_3$." *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 $WO_3$." *APS March Meeting.* March 13-18, 2017. New Orleans, LA.

- **W. Wang**, A. Janotti, C.G. Van de Walle. "Phase Transformations upon doping in $WO_3$." *MSE Congress.* Sept 27-29, 2016. Darmstadt, Germany

- **W. Wang**, A. Janotti, C.G. Van de Walle. "Phase Transformations upon doping in $WO_3$." *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 $WO_3$." *145$^{th}$ 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 $WO_3$." *28$^{th}$ ICDS.* Espoo, Finland. July 27-31, 2015.

- **W. Wang**, A. Janotti, C.G. Van de Walle. "Uncovering the connection between dopants and defects in $WO_3$." *MRS Spring Meeting.* San Francisco, CA. April 6-10, 2015.

- **W. Wang**, A. Janotti, C.G. Van de Walle. "Understanding the Oxygen Vacancy in $WO_3$." *APS March Meeting*, San Antonio, TX. March 2-6, 2015. (Session S9)

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## Outreach/DEI Conferences

- (pending) **W. Wang**, "Navigating the Job Market as a Physics or STEM degree holder (in the era of COVID)," University of Illinois, Urbana-Champaign, Depart. of Physics as APS Career Mentoring Fellow. 4 Dec 2020
- **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.

## Seminars/Posters

- **W. Wang** and J.X. Shen. "Rapid fire MPI/OpenMP: A brief introduction to code parallelization." UCSB Graduate Simulation Seminar Series Workshop. Sept. 2017.
- **W. Wang**. "Atom by atom: Understanding defects using first-principles calculations." UCSB Graduate Simulation Seminar Series. Aug 2016. Awarded and voted top seminar given.
- **W. Wang**, M. Swift, K. Krishanaswamy, Y. Kang, B. Himmetoglu, C.G. Van de Walle. "Transport in complex oxides: understanding mobility from first principles." UCSB MROP. Feb. 2017.
- **W. Wang**, A. Janotti, C.G. Van de Walle. "Understanding the Spontaneous Phase Transformation in $WO_3$." UCSB MROP. Feb 2015

## Service/Outreach Activities

**Reviewer:** *Chem. Mater.; JACS; J. Chem. Phys. Lett.; Phys. Rev. Mater.; J. Appl. Phys.; Phys. Status Solidi B; J. Chem. Theory. Comp.*

**APS Forum for Early Career Scientists** 2020-current
- Member-at-large

**APS Career Mentoring Fellow** 2020

**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 for diversity and inclusion efforts quarterly

**UCSB Science Line** Spring 2014-Spring 2018
- Certificate of Excellence for answering 2015, 2016

**MIT AX of Alpha Phi Omega** (national, co-ed service fraternity) Fall 2010-Spring 2013
- Service VP (Fall 2011), Membership Chair (Fall 2012), Pledge VP (Spring 2013)
- Chapter Distinguished Service Key (Spring 2013)

**MIT Tau Beta Pi Engineering Honor Society** 2012-2013