

Wennie Wang

wwwennie@uchicago.com | wenniewang.com | github.com/wwwennie

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

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

Research Experience

University of Chicago, Pritzker School of Molecular Engineering (PME) Chicago, IL
Postdoctoral Scholar, Adviser: Giulia Galli Summer 2018 - current

- Using density functional theory (DFT) and many-body theory to understand surfaces and interfaces of complex oxides for water-splitting technologies and neuromorphic computing

UCSB Materials Department Santa Barbara, CA
Graduate Student Researcher, Adviser: Chris G. Van de Walle Fall 2013 – Spring 2018

- Using density functional theory (DFT) for understanding defects and impurities in electronic materials, including elucidating mechanism(s) of electrochromism, mobility and transport, and influence of defects on electronic properties in complex oxides

MIT NECST Lab Cambridge, MA
Student researcher, Adviser: Brian Wardle Fall 2011- Spring 2013

- Mechanical characterization of carbon nanotube fiber reinforced composites—Department Aeronautics and Astronautics; [thesis, in collaboration with Metis Corp.]

Fraunhofer Institute CSP Halle (Saale), Germany
Student Intern, Adviser: Stefan Schoenfelder Summer 2012

- Characterization and modeling of mechanical properties and fracture mechanics of solar cell metallization systems using theoretical modeling in comparison with 4-point bending tests and fractography imaging
- Top 10 paper submission to SiliconPV 2013 conference

Siemens AG Berlin, Germany
Student intern, Adviser: Matthias Lang Summer 2011

- Designed and optimized stator of radial magnetic bearings using finite element analysis

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 that do not use Shor's algorithm; presented findings to faculty;
- Built demonstrations for the honors Mechanics class, such as a giant Newton's cradle out of bowling balls

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

Wennie Wang

wwwennie@uchicago.com | wenniewang.com | github.com/wwwennie

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
- SPIE MKS Instruments Research Excellence Travel Award Winter 2018
- MRS Fall 2017 Graduate Student Award finalist (Silver Award) Fall 2017
- UCSB GSA Excellence in Teaching Award (nominated) Spring 2016
- APS Ovshinsky Travel Award Honorable Mention Winter 2016
- UCSB MRL Travel Grant Winter 2018, Fall 2017, Winter 2017, Summer 2016, Summer 2015
- UIUC MCC Travel Grant Summer 2015
- UCSB MRL Travel Fellowship to DMMM1 Conference on diversity Summer 2014

Publications

*= equal contribution; ^ = undergraduate researcher

Upcoming Publications

- M. Favaro, **W. Wang**, E. Chen[^], K.-S. Choi, G. Galli, D. Starr. “A joint experimental and first-principles investigation on hydroxylation of the BiVO₄ (010) surface.” (in preparation)
- (invited) **W. Wang**, A. Hilbrands, C. Zhou, E. Chen[^], M. Liu, K-S. Choi, G. Galli. “Open questions and strategies towards a renaissance of integrated experiment and theory for photoelectrodes in water splitting.” *J. Mater. Chem. A* (in preparation)
- (invited) **W. Wang**, A. Radmilovic, K.-S. Choi, G. Galli. “Integrating computation and experiment to investigate photoelectrodes for solar water splitting at the microscopic scale” *Acc. Chem. Res.* (submitted)

Peer-reviewed Publications

- 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/acs.aem.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]

Wennie Wang

wwwennie@uchicago.com | wenniewang.com | github.com/wwwennie

- **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]

Patents

- Inventors: W. Wang, M. Lang
German Patent: 2011E22406 DE/ 201206715. "*Actives Radialmagnetlager mit Polen aus hochpermeablen 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

Technical Talks

- **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 $BiVO_4$ (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 $BiVO_4$ (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 $BiVO_4$." MRS Fall Meeting. December 1-6, 2019. Boston, MA.

Wennie Wang

wwwennie@uchicago.com | wenniewang.com | github.com/wwwennie

- **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.
- **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 Conferences

- **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.

Seminars/Posters

- **W. Wang**. "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. Krishnaswamy, 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 WO₃." UCSB MROP. Feb 2015

Wennie Wang

wwwennie@uchicago.com | wenniewang.com | github.com/wwwennie

Teaching Experience

University of Chicago Materials Research Science and Engineering Center

Chicago, IL

Lead instructor

Fall 2018- current

- Create, organize and teach science colloquium at Lindbloom High School in collaboration with graduate students
- Mentor in pedagogy for graduate instructors; [weblink]

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 MAT 228 Computational Materials

Santa Barbara, CA

Teaching Assistant

Spring 2017

- Graduate level course covering wide range of methods for simulating materials, with Prof. Chris Van de Walle

UCSB MAT 211A Engineering Quantum Mechanics I & II

Santa Barbara, CA

Teaching Assistant

Winter 2017

- Graduate level course for all incoming students, with Prof. Chris Van de Walle

UCSB MAT 200B Electronic and Atomic Structure of Materials

Santa Barbara, CA

Teaching Assistant

Winter 2015

- Winter 2015 quarter graduate level course for all incoming students, with Prof. Michael Chabiny

MIT 3.091 Introduction to Solid State Chemistry

Cambridge, MA

Teaching Assistant

Fall 2012

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-current

APS Career Mentoring Fellow

2020, 2021

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