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**University of Texas at Austin (UT)** 

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<sub>3</sub>

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

### **Publications**

\*= equal contribution; ^ = undergrad, #= corresponding author, <u>underlined</u> = Wang Mat Group member Submitted/Under Review

- <u>J.-L. Ng</u>, **W. Wang**<sup>#</sup>. "Assessment of density functional theory methods on bulk and electronic properties of β-NiOOH Structural Models." *Submitted* (2025).
- L.A. Smith, J.E. Eichler, <u>S.G. Lim</u>, M.N. Davenport, H. Leonard, E.K. Yang, Y. Karbalaeemorad, B.D. Freeman, W. Wang, R.P.P.L. Ribeiro, C.B. Mullins. "Ethan-selective Activated Nitrogen-doped Carbons for Ethane-Ethylene Separation." *Submitted*. (2025).
- C.E. Chukwuneke, K. Kawashima, T.P.A Nguyen, G. Ruiz, J.P. Smith, R.A. Marquez, J.T. Bender, <u>J.L. Ng</u>, X. Zhan, **W. Wang**, D.J. Milliron, M. J. Rose, C.B. Mullins. "Doping and Nitridation Effects on Nickel-based MOF for Water Oxidation." *Under revision*. (2025).
- <u>B. Kumela</u>, <u>R. Anvari</u>, **W. Wang**<sup>#</sup>. "Interfacial Electronic Structure Modulation by Facet Orientation and Sulfur Vacancies in CdS/MoS<sub>2</sub> Heterojunctions" *Under revision*. [chemrxiv] (2025).
- E. Murhula, \*W. Wang\*, G.L. Dzemua, <u>S.G. Lim</u>, G. Schatte, L. Zuin, C.E. Gibson\*. "Unveiling the Amphoteric Surface Reactivity of Montebrasite using Spectroscopic and First-Principles Methods" *Under revision* (2025).
- R. Anvari, D. Akinwande, **W. Wang**.\* "Effect of electric field on the hysteresis and switching behavior of the MoS<sub>2</sub>/Au(111) heterojunction." *Under revision*. [chemrxiv] [zenodo data] (2025).

## Peer-reviewed

- J. Fatheema, L. Liang, <u>B.H. Lee</u>, **W. Wang**, D. Akinwande, "First-Principles Investigation of the Resistive Switching Energetics in Monolayer MoS<sub>2</sub>: Insights into Metal Diffusion and Adsorption." *Accepted: npj 2D Materials and applications* (2023 IF: 9.2). (2025).
- <u>B.H. Lee</u>, J. Fatheema, D. Akinwande, **W. Wang.** "Understanding and predicting trends in adsorption energetics in monolayer transition metal dichalcogenides." *npj 2D Materials and Applications*, 9, 61 (2025) (2023 IF: 9.2). [pre-print] [zenodo data] [doi: 10.1038/s41699-025-00579-9]
- R. Anvari, **W. Wang**<sup>#</sup>. "Nature of point defects in monolayer MoS<sub>2</sub> and the MoS<sub>2</sub>/(111)-Au heterojunction." *J. Appl. Phys* (2023 IF = 2.7). 135, 174304 (2024). *Defects in Semiconductors 2024* special edition. [doi: 10.1063/5.0205981] [arXiv]

#### Pre-UT

- G. Melani, **W. Wang**, F. Gygi, K.-S. Choi. G. Galli. "Effects of solvation and temperature on the energetics of BiVO4 surfaces with varying composition for solar water splitting." *ACS Energy Letters* (2023 IF = 19.3). 9, 10, 5166-5171 (2024). [doi: **10.1021/acsenergylett.4c01913**] [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 BiVO<sub>4</sub> (010) surface." *J. Am. Chem. Soc.* (2023 IF = 15.4), 144, 37, 17173–17185 (2022) [doi: 10.1021/jacs.2c07501].

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- (invited) **W. Wang**, A. Radmilovic, K.-S. Choi, G. Galli. "Investigating photoelectrodes for solar water splitting at the microscopic scale" *Acc. Chem. Res* (2021 IF = 24.4). 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 IF = 4.3). (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 BiVO<sub>4</sub>." *Nature Energy* (2021 IF = 67.4). 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 PbCrO<sub>4</sub>photoanode perform as well as isoelectronic BiVO<sub>4</sub>?" *ACS Appl. Energy Mater* (2020 IF = 8.7). (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.* (2020 IF = 3.3) 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<sub>4</sub>." *Chemistry of Materials* (2020 IF = 6.1). 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<sub>3</sub>." *Phys. Rev. B* (2020 IF = 4.0). **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* (2018 IF = 16.3). 3, 2329-2334 (2018). [doi: 10.1021/acsenergylett.8b01297]
- **W. Wang**<sup>#</sup>, H. Peelaers, J.X. Shen, C.G. Van de Walle. "Carrier-induced absorption as a mechanism for electrochromism in WO<sub>3</sub>." *MRS Communications* (2018 IF = 1.9). **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<sub>3</sub>." 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<sub>3</sub>." *J. Chem. Phys.*, 146, 214504 (2017 IF = 2.8) (2017), [doi: 10.1063/1.4984581]
- **W. Wang**, A. Janotti, C.G. Van de Walle. "Role of oxygen vacancies in crystalline WO<sub>3</sub>." *J. Mat Chem. C*, 4, 6641 6648 (2016) (2017 IF = 5.2), [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* (2014 IF = 6.3). 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* (2014 IF = 3.5). 100, 128-135 (2014). [doi: 10.1016/j.compscitech.2014.06.003]

#### Patents

Inventors: <u>W. Wang</u>, 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

#### **Awards**

| • | APS Maria Goeppert Mayer Award [link]   | 2025        |
|---|---|-------------|
| • | APS Reviewer Excellence Award (PRX Energy) [link]                                     | 2024        |
| • | APS 5 Sigma Physicist Award (science policy advocacy)                                 | 2024        |
| • | ACS PRF Doctoral New Investigator   | 2024        |
| • | 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 |
|   |   |             |

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| •      | MRS Fall 2017 Graduate Student Award finalist (Silver Award)            | Fall 2017   |
|--------|---|-------------|
| •      | APS Ovshinsky Travel Award Honorable Mention                            | Winter 2016 |
| Fellov | vships  |             |
| •      | 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 |
|        |   |             |

#### Technical Talks/Presentations

#### **Invited**

- **W. Wang.** "Leveraging defects and interfaces based on low-dimensional materials for memristors." International Conference on Defects in Semiconductors (ICDS). Sept 14-19, 2025. Shanghai, China.
- W. Wang. "Microscopic insights to resistive switching mechanisms in heterojunctions with monolayer materials"
   Sept 1 Sept 3, 2025. Poznań, Poland.
- **W. Wang.** "Computational and Theoretical Insights on Materials Defects and Low-dimensional Systems for Energy Sustainability" MIT DMSE Seminar. April 1, 2025. Cambridge, MA. [link]
- **W. Wang.** "Harnessing materials imperfections for energy sustainability: understanding and designing defects in semiconductors" APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- W. Wang. "Physical models and computational insights for adsorption-related technologies
- for energy sustainability." University of Aveiro (Jan 15, 2025), University of Porto (Jan 16, 2025), International Iberian Nanotechnology Laboratory (INL, Jan 17, 2025). UT-Portugal exchange.
- **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. July17-21, 2023.
- **W. Wang.** "Bridging first-principles calculations with experiment: Insights from case studies on (photo)electrochemical systems." 152<sup>nd</sup> TMS Meeting and Exhibition. 22 March 2023. San Diego, CA

#### Pre-UT presentations

- **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 Angles, CA.
- **W. Wang**, H. Peelaers, J.-X. Shen, C.G. Van de Walle. "Mechanisms of electrochromism in WO<sub>3</sub>." *SPIE-Photonics West: Oxide-based Materials and Devices International Conference IX*. Jan 27-Feb 1, 2018. San Francisco, CA.

#### **Contributed:**

• (poster) E. Murhula, **W. Wang**, L. Babedi, C. Gibson. "Experimental and computational study of the surface chemistry and floatability of montebrasite." 12<sup>th</sup> International Flotation Conference. Nov 17-20, 2025. Cape Town, South Africa.

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- E. Murhula, **W. Wang**, C. Hill-Svehla, L. Babedi, C. Gibson. "The Role of Na2CO3 in the Selective Flotation of Ca-activated Spodumene and Quartz." 12<sup>th</sup> International Flotation Conference. Nov 17-20, 2025. Cape Town, South Africa.
- A.E. Fernando Milton, K. Kawashima, Y.J. Son, W.J. Chang, R.R. Vaidyula, <u>J.L. Ng</u>, V.C. Negandhi, D.T. Collins, N.L. Serrat, D.D. Thakkar, **W. Wang**, D.J. Milliron, and C. Buddie Mullins. "In-Situ SERS Study of Ni(OH)<sub>2</sub> on FTO During the OER Using Electrochemically Deposited Au Nanoparticles and a 3D-Printed Raman Cell" 248th ECS Meeting. Oct 12-16, 2025. Chicago, IL.
- E. Murhula, **W. Wang,** K. Beatty, L. Zuin, C. Gibson. "Core-level spectroscopy and first-principles study of spodumene and montebrasite under flotation conditions." Uranium, Potash, and Lithium International Conference. September 8-11, 2025. Saskatoon, Saskatchewan, Canada.
- J. Fatheema, L. Liang, **W. Wang**, D. Akinwande. "First-principles investigation of the resistive switching mechanism in monolayer MoS<sub>2</sub> Insights into metal diffusion and adsorption." MRS Spring Meeting & Exhibit. April 11, 2025. Seattle, WA. EL03: Progress in van der Waals Heterostructures for Sustainable Electronics.
- **W. Wang.** "Influence of structural disorder in oxide electrocatalysts through first-principles calculations." APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- X. Chang, W. Wang. "Understanding the role of charge transfer states in singlet fission in Perylenediimide crystals." APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- (poster) X. Chang, W. Wang, F. Spano. "Absorption and photoluminescence in π-stacks of donor-acceptor-donor chromophores: A Frenkel-Holstein Approach." APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- R. Anvari, W. Wang. "Effect of electric field on the electronic structure and switching behavior of MoS<sub>2</sub>/Au(111) heterostructures." APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- (poster) <u>R. Anvari</u>, **W. Wang.** "Switching dynamics of MoS<sub>2</sub>/Au(111) heterostructures." APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- <u>B.H. Lee</u>, J. Fatheema, D. Akinwande, **W. Wang**. "Understanding and predicting adsorption energetics on monolayer transition metal dichalcogenides." APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- <u>J.-L. Ng</u>, **W. Wang.** "Assessment of density functional theory methods on bulk and electronic properties of β-NiOOH Structural Models." APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- <u>B. Kumela</u>^, <u>R. Anvari</u>, **W. Wang.** "First-principles study on CdS/MoS<sub>2</sub> heterostructures for water-splitting reactions." APS Global Physics Summit. March 16-21, 2025. Anaheim, CA.
- K. Kawashima, <u>J.-L. Ng</u>, 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)<sub>2</sub> and Ni(OH)<sub>2</sub> Electrocatalysts." ECS PRiME. Oct 6-11, 2024. Honolulu, HI.
- (poster) <u>J.-L. Ng</u>, K. Kawshima, Y-J. Son, J. Resasco, C.B. Mullins, W. Wang. "Integrated computational and experimental study of Nickel Oxyhydroxides for water splitting." UT Austin ECS Texas Section Symposium. September 14, 2024.
- (poster) <u>B.H. Lee</u>, **W. Wang.** "First-principles investigation into the adsorption monolayer transition metal dichalcogenides." GRC Defects in Semiconductors: Defects, from Fundamental Properties to Designed Functionalities. Aug 4-9, 2024. Newry, Maine.
- <u>J.-L. Ng</u>, 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.
- <u>J-L. Ng</u>, <u>A. Anderson</u>^, **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 MoS<sub>2</sub>-based memristors." 2024 APS March Meeting. March 3-8, 2024. Minneapolis, MN.
- <u>A.M. Anderson</u>^, **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.

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- <u>J.-L. Ng</u>, 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.

#### **Pre-UT Presentations**

- **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 BiVO<sub>4</sub> (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 BiVO<sub>4</sub> 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 BiVO<sub>4</sub> (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<sub>4</sub>." 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 BiVO<sub>4</sub>." 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 WO<sub>3</sub>." *APS March Meeting*. March 5-9, 2018. Los Angles, CA.
- **W. Wang**, H. Peelaers, J.-X. Shen, C.G. Van de Walle. "Influence of Structural Distortions on Optical Absorption in WO<sub>3</sub>." *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<sub>3</sub>." *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<sub>3</sub>." *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<sub>3</sub>." *MSE Congress*. Sept 27-29, 2016. Darmstadt, Germany
- **W. Wang**, A. Janotti, C.G. Van de Walle. "Phase Transformations upon doping in WO<sub>3</sub>." *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<sub>3</sub>." *145<sup>th</sup> 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<sub>3</sub>." *28*<sup>th</sup> *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<sub>3</sub>." *MRS Spring Meeting*. San Francisco, CA. April 6-10, 2015.

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• **W. Wang**, A. Janotti, C.G. Van de Walle. "Understanding the Oxygen Vacancy in WO<sub>3</sub>." *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"
- **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 GS<sup>3</sup>: 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. *145<sup>th</sup> 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 210: Introduction to Computing

Austin, TX

Instructor
 Undergraduate first-year course: units, mass balance, processes in chemical engineering

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

Austin, TX Fall 2024

Instructor

## University of Texas at Austin CHE 350: Chemical Engineering Materials

Austin, TX

Instructor

Spring 2022 -- Spring 2024

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

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- broken]

Fall 2018-Fall 2021

 Modern Materials Technologies: Semester-long weekly colloquium for high school students in the Chicago Public School System

#### **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

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## Service Experience

**Journal Reviews:** Nature Energy; Nature Synthesis; Nature Commun.; ACS Nano; ACS Energy Letters; J. Am. Ceramic Soc.; ACS Applied Electronic Materials; ACS Electronics; Chem. Mater.; ACS Catalysis; Chem. Phys.; Phys. Rev Letters; Appl. Phys. Lett.; J. Chem. Phys. Lett.; J. Phys. Chem.; Phys. Rev X; Phys. Rev. Energy; Phys. Rev. Mater.; J. Appl. Phys.; Phys. Status Solidi B; J. Mater. Chem. C; New J. Chem.; J. Chem. Theory. Comp.

**Editorial boards:** Chem & Bio Engineering Journal (ACS, ECAB member, 2024-2026); ACS Applied Electronic Materials Early Career Board member (Jan 2025 – Jan 2027)

**Grants Reviews:** DOE RENEW (2022), NSF GRFP (2023, 2024), AI4Materials Design Workshop (2023), NSF CBET Catalysis (2023, 2024), DOD NSDEG (2024), ACS PRF (2024, 2025)

**Department Service:** OXE Faculty advisor (Spring 2023-); Junior Faculty mentor (2023-); Faculty Search (2023), Graduate Admissions Committee (2022, 2023, 2024); ChE Best Paper Committee (chair: Kent Zheng 2024, 2025); ChE Best Paper Committee chair (2026)

University Service: AI faculty cluster hire (2024) (Chair: David Allen; main chair: Jamie Warner),

**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); TMS Computational Physics of Materials Committee (2023-); APS Maria Goeppert Mayer Award selection committee (2025);

#### **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

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

Vita

Wennie Wang is a computational materials scientist and current assistant professor in the McKetta Department of Chemical Engineering at the University of Texas at Austin. She earned her B.S. degree in Materials Science and Engineering from the Massachusetts Institute of Technology in 2013, followed by her Ph.D. in Materials at the University of California, Santa Barbara in 2018 and a postdoctoral appointment at the University of Chicago in the Pritzker School of Molecular Engineering. Her research focuses on the usage and deployment of first-principles computational methods for studying the optical and electronic properties of semiconductors, with a particular emphasis on defects in transition metal compounds. The Wang Materials Group focuses on combining electronic structure calculations and simulated spectroscopy, working closely with experimentalists towards energy sustainability applications. Her group's work has been recognized through the NSF GRFP, UCSB Energy Institute, the MRS Fall Silver Graduate Student Award (2017), the APS Ken Hass Outstanding Student Paper Award runner-up (2018), and 2025 APS Maria Goeppert Mayer Award. Wennie also served as chair of the APS Forum for Early Career Scientists (FECS) and is an APS Career Mentors Fellow, of which her efforts have been recognized with a 2024 APS 5 Sigma Physicist Award.