

# Mingjian Wen

ASSISTANT PROFESSOR, CHEMICAL AND BIOMOLECULAR ENGINEERING  
UNIVERSITY OF HOUSTON

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## Professional Experience

### University of Houston

Sept 2022 - Present

**Assistant Professor**, Department of Chemical and Biomolecular Engineering

### Tianjin University

Jul 2012 - Jul 2013

**Research Assistant**, School of Chemical Engineering and Technology

## Education & Academic Training

### Lawrence Berkeley National Laboratory

Aug 2019 - Aug 2022

**Postdoc**, Energy Storage and Distributed Resources Division

Advisor: Prof. Kristin A. Persson

### University of Minnesota, Twin Cities

Aug 2013 - Jul 2019

**Ph.D.**, Aerospace Engineering and Mechanics

Advisor: Prof. Ellad B. Tadmor

### Tianjin University

Sept 2008 - Jul 2012

**B.S.**, Chemical Engineering

## Honors & Awards

Alternative Textbook Incentive Award	University of Houston	2023
Presidential Frontier Faculty Fellow	University of Houston	2022
Travel Grant of Machine Learning for Solids Workshop	Los Alamos National Laboratory	2019
Travel Grant of Uncertainty Quantification Conference	U.S. Association for Computational Mechanics	2019
Doctoral Dissertation Fellowship	University of Minnesota	2018
National Scholarship for Graduate Students	Ministry of Education of China	2012
National Scholarship for Undergraduate Students	Ministry of Education of China	2010 & 2011
Outstanding Graduate from class of 2012	Tianjin University	2012

## Teaching

### CHEE 6397: Data-driven Materials Modeling

Fall 2023

Instructor

- Graduate-level elective course
- Machine learning for chemical and materials sciences

### CHEE 3300: Materials Science & Engineering

Spring 2023

Instructor

- Core Chemical Engineering undergraduate course

### Materials Project Workshop

Aug 2021

Instructor

- Designed advanced Python tutorial materials and exercises
- Taught the interactive course virtually via an online teaching platform (recording available on [YouTube](#))

## Teaching Assistant

- Taught recitation course for *Mechanics of Materials* (AEM 3031)
- Designed homework and quizzes together with the instructor for *Aerospace Structures* (AEM 4501)

## Research Funding

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1. LEAPS-MPS: Machine learning-guided identification of mechanically stabilizing solid-state electrolytes, \$250,000, NSF, PI: Mingjian Wen, 2023–2025.

## Students

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## POSTDOCTORAL SCHOLARS

Santosh Adhikari, *Long-range interactions in atomistic systems*, 2023 –

Jin Dai, *Dendrite growth and control in solid-state batteries*, 2023 –

## PH.D. STUDENTS

Wei-Fan Huang, ChBE, *Inorganic electrolytes for solid-state batteries*, 2023 –

Emmanuel A. Olanrewaju, ChBE, *Stability and synthesizability of zeolite catalysts*, 2023 –

Dale G. Green, ChBE, (co-advised with Prof. Lars Grabow), *Ether catalysis*, 2023 –

## UNDERGRADUATE STUDENTS

Robert H. Brown, ChBE, *Awarded UH Summer Undergraduate Research Fellowship*, 2023 –

Chris Mobley, ChBE, *Awarded UH Provost's Undergraduate Research Scholarship*, 2023 –

Heer Loungani, Houston Community College, *Awarded LSAMP Summer Fellowship*, Summer 2023

## Professional Affiliations

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American Institute of Chemical Engineers (AIChE), *Member*

2022 - present

American Chemistry Society (ACS), *Member*

2020 - 2022

American Physical Society (APS), *Member*

2020 - 2021

## Professional Service

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## CONFERENCE SYMPOSIA

**AIChE CAST, Session Chair**, Advances in Machine Learning and Intelligent Systems 2023

**AIChE MESD, Session Chair**, Inorganic Materials for Electrochemical Energy Storage 2023

**AIChE ESF, Session Co-chair**, Electrochemical Fundamentals 2023

## REVIEWER FOR FUNDING AGENCIES

*Natural Sciences and Engineering Research Council of Canada (NSERC)*

## REVIEWER FOR JOURNALS AND CONFERENCES

*Physical Review Letters*

*Physical Review B*

*Physical Review Materials*

*Nature Communications*

*Applied Physics Reviews*

*Machine Learning: Science and Technology*

*Digital Discovery*

*Journal of Applied Physics*

*Journal of Physics D: Applied Physics*

*NeurIPS*

*2D Materials*

*Journal of Chemical Information and Modeling*

*IOP Nanotechnology*

## Public Service

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Houston Energy Day, *UH exhibits co-organizer*

2022

## Publications

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## PREPRINTS

3. **M. Wen**, MK Horton, JM Munro, P Huck, and KA Persson, "A universal equivariant graph neural network for the elasticity tensors of any crystal system," *arXiv:2307.15242*, 2023.
2. S Vijay, MC Venetos, EWC Spotte-Smith, AD Kaplan, **M Wen**, and KA Persson, "CoeffNET: Predicting activation barriers through a chemically-interpretable, equivariant and physically constrained graph neural network," *ChemRxiv*, 2023.
1. Z Shui, P Karypis, DS Karls, **M Wen**, EB Tadmor, and G Karypis, "Fine-tuning language models on multiple datasets for citation intention identification," *under review*, 2023.

## PEER-REVIEWED PAPERS

18. MC Venetos, **M Wen**, and KA Persson, "Machine learning full NMR tensors with equivariant graph neural networks," *Journal of Physical Chemistry: A*, 127, 10, 2388–2398 (2023).
17. **M Wen**, EWC Spotte-Smith, SM Blau, MJ McDermott, AS Krishnapriyan, and KA Persson, "Chemical reaction networks and opportunities for machine learning," *Nature Computational Science*, 3, 12–24 (2023).
16. Z Shui, DS Karls\*, **M Wen**\*, IA Nikiforov, EB Tadmor, and G Karypis, "Injecting domain knowledge from empirical interatomic potentials to neural networks for predicting material properties," *36th Conference on Neural Information Processing Systems (NeurIPS)*, 2022.
15. Y Kurniawan, CL Petrie, MK Transtrum, EB Tadmor, RS Elliott, DS Karls, and **M Wen**, "Extending OpenKIM with an uncertainty quantification toolkit for molecular modeling," *e-Science*, 367–377 (2022).
14. Y Kurniawan, CL Petrie, KJ Williams, MK Transtrum, EB Tadmor, RS Elliott, DS Karls, and **M Wen**, "Bayesian, frequentist, and information geometry approaches to parametric uncertainty quantification of classical empirical potentials," *Journal of Chemical Physics*, 156, 214103 (2022).
13. **M Wen**, SM Blau, XXie, S Dwaraknath, and KA Persson, "Improve machine learning performance on small chemical reaction data with unsupervised contrastive pretraining," *Chemical Science*, 13, 1446–1458 (2022).
12. **M Wen**, Y Afshar, RS Elliott, and EB Tadmor, "KLIFF: A framework to develop physics-based and machine learning interatomic potential," *Computer Physics Communication*, 108218 (2021).
11. X Xie, EWC Spotte-Smith, **M Wen**, H Patel, SM Blau, and KA Persson, "Data-driven prediction of formation mechanisms of lithium ethylene monocarbonate with an automated reaction network," *Journal of the American Chemical Society*, 143, 13245 (2021).
10. EWC Spotte-Smith, SM Blau, X Xie, H Patel, **M Wen**, B Wood, S Dwaraknath, and KA Persson, "Quantum chemical calculations of lithium-ion battery electrolyte and interphase species," *Scientific Data*, 8, 203 (2021).
9. **M Wen**, SM Blau, EWC Spotte-Smith, S Dwaraknath and KA Persson, "BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules," *Chemical Science*, 12, 1858–1868 (2021).
8. **M Wen** and EB Tadmor, "Uncertainty quantification in molecular simulations with dropout neural network potentials," *npj Computational Materials*, 6, 124 (2020).
7. **M Wen** and EB Tadmor, "Hybrid neural network potential for multilayer graphene," *Physical Review B*, 100, 195419 (2019).
6. **M Wen**, S Carr, S Fang, E Kaxiras, and EB Tadmor, "Dihedral-angle-corrected registry-dependent interlayer potential for multilayer graphene structures," *Physical Review B*, 98, 235404 (2018).
5. **M Wen**, SN Shirodkar, P Plecháč, E Kaxiras, and EB Tadmor, "A force-matching Stillinger-Weber potential for MoS<sub>2</sub>: Parameterization and Fisher information theory based sensitivity analysis," *Journal of Applied Physics*, 122, 244301 (2017).
4. **M Wen**, J Li, P Brommer, JP Sethna, RS Elliott, and EB Tadmor, "A KIM-compliant *potfit* for fitting sloppy interatomic potentials: Application to the EDIP model for silicon," *Modelling and Simulation in Materials Science and Engineering*, 25, 014001 (2017).
3. **M Wen**, SM Whalen, RS Elliott, and EB Tadmor, "Interpolation effects in tabulated interatomic potentials," *Mod-*

*elling and Simulation in Materials Science and Engineering*, 23, 074008 (2015).

2. H Li, **M Wen**, G Chen, W Yu, and X Chen, "Constitutive modeling for the anisotropic uniaxial ratcheting behavior of Zr-4 alloy at room temperature," *Journal of Nuclear Materials*, 443, 152-160 (2013).
1. **M Wen**, H Li, D Yu, G Chen, and X Chen, "Uniaxial ratcheting behavior of Zircaloy-4 tubes at room temperature," *Materials Design*, 46, 426-434 (2013).

## THESIS

1. **M Wen**, "Development of interatomic potentials with uncertainty quantification: applications to two-dimensional materials," *Ph.D. thesis, University of Minnesota*, Minneapolis, MN, USA, July 2019.

✉Corresponding author

\*Equal contribution

## Departmental Seminar & Invited Talks

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8. Accelerated Materials Design Driven by Machine Learning, *3M*, Saint Paul, MN, Oct. 12, 2023.
7. Accelerated Materials Design Driven by Machine Learning, *Department of Chemical and Biomedical Engineering*, Cleveland State University, Oct. 5, 2023.
6. Accelerated Materials Design Driven by Machine Learning, *HPE Data Science Institute*, University of Houston, Sept. 8, 2023.
5. Reliable molecular simulations using uncertainty-quantified machine learning potentials, *11th Mach Conference*, Baltimore, MD, Apr. 4-7, 2023.
4. Interplay between mechanics and chemistry in battery materials, *Department of Mechanics and Aerospace Engineering*, Southern University of Science and Technology, Virtual, Feb. 15, 2022.
3. Computational study of the mechanical behaviors of 2D materials, *School of Aerospace Engineering*, Huazhong University of Science and Technology, Virtual, Dec. 28, 2021.
2. Computational study of the mechanical behaviors of 2D materials, *School of Mechanical Science & Engineering*, Huazhong University of Science and Technology, Virtual, Dec. 27, 2021.
1. Computational study of the mechanical behaviors of 2D materials, *College of Science*, Harbin Institute of Technology—Shenzhen, Virtual, Dec. 10, 2021.

## Contributed Presentations

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12. Machine learning full elastic tensors with equivariant neural networks, *2023 SES Annual Technical Meeting*, Minneapolis, MN, Oct. 8-11, 2023.
11. Reliable molecular simulation using uncertainty-quantified machine learning potentials, *2023 SES Annual Technical Meeting*, Minneapolis, MN, Oct. 8-11, 2023.
10. Machine learning full elastic tensors of inorganic materials with equivariant neural networks, *2023 AIChE Annual Meeting*, Orlando, FL, Nov. 5-10, 2023.
9. Accurate prediction of bond dissociation energies for molecules of any charge, *ACS Spring 2021*, Virtual, Apr. 5-30, 2021.
8. Uncertainty quantification in atomistic simulations with dropout neural network potentials, *APS March Meeting*, Virtual, Mar. 2-6, 2020.
7. Uncertainty quantification in atomistic simulations with dropout neural network potentials, *Workshop on Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, NM, Feb. 18-20, 2019.
6. Uncertainty quantification in atomistic simulations with dropout neural network potentials, *U.S. Association for Computational Mechanics Conference on Uncertainty Quantification in Computational Solid and Structural Materials Modeling*, Baltimore, MD, Jan. 17-18, 2019.

5. Machine learning interatomic potentials for multilayer graphene structures, *Conference on Emerging Ideas in Mechanics and Materials Science*, Minneapolis, MN, Oct. 19, 2018.
4. Interatomic potential models for 2D heterostructures, *18th U.S. National Congress for Theoretical and Applied Mechanics (USNC/TAM)*, Chicago, IL, Jun. 7, 2018.
3. Development of interatomic potentials for 2D heterostructures, *AEM Mechanics Research Seminar*, University of Minnesota, Minneapolis, MN, Nov. 21, 2017.
2. Stillinger-Weber potential for MoS<sub>2</sub>: parameterization and sensitivity analysis, *Workshop on Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials*, Harvard University, Cambridge, MA, Dec. 1-2, 2016 (poster).
1. Fitting interatomic models for layered heterostructures using OpenKIM, *Workshop on Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials*, Harvard University, Cambridge, MA, Dec. 7-8, 2015 (poster).

## Open-source Codes

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7. MatTen: Materials Tensor Structure-property Predictor, author, <https://github.com/wengroup/matten>
6. KLIF: KIM-based Learning-Integrated Fitting Framework, author, <https://kliff.readthedocs.io>
5. LAMMPS “pair\_style drip” for the DRIP Potential, author, [https://lammps.sandia.gov/doc/pair\\_drip.html](https://lammps.sandia.gov/doc/pair_drip.html)
4. kimpy: a Python interface to the KIM-API, author, <https://github.com/openkim/kimpy>
3. BondNet: a Graph Neural Network Model for the Prediction of Bond Dissociation Energies, author, <https://github.com/mjwen/bondnet>
2. RxnRep: Self-supervised Contrastive Pretraining for Chemical Reaction Representation, author, <https://github.com/mjwen/rxnrep>
1. Atomic Simulation Environment (ASE) KIM Calculator, contributor, in collaboration with Ellad Tadmor and Dan Karls, <https://wiki.fysik.dtu.dk/ase/ase/calculators/kim.html>