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)

University of Minnesota, Twin Cities *Aug 2013 - Jun 2015*

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

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

Students

Postdoctoral Scholars

Santosh Adhikari, 2023 –

Ph.D. Students

Wei-Fan Huang, ChBE, 2023 –
Emmanuel A. Olanrewaju, ChBE, 2023 –
Dale G. Green, ChBE, (co-advised with Prof. Lars Grabow), 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

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

Conference Symposiums

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
Nature Communications
Digital Discovery
NeurIPS
Physical Review B
Applied Physics Reviews
Journal of Applied Physics
2D Materials
Physical Review Materials
Machine Learning: Science and Technology
Journal of Physics D: Applied Physics
IOP Nanotechnology

Public Service

Houston Energy Day, *UH exhibits co-organizer* *2022*

Publications

Google Scholar: `https://scholar.google.com/citations?user=RXLH5k4AAAAJ`

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, "CoffNET: Predicting activation barriers through a chemically-interpretable, equivariant and physically constrained graph neural network," *under review,* 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, X Xie, 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_2: 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," *Modelling 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

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

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_2: 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

7. MatTen: Materials Tensor Structure–property Predictor, author, `https://github.com/wengroup/matten`
6. KLIFF: 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`
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`