Mingjian Wen

Assistant Professor, Chemical and Biomolecular Engineering
University of Houston

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Education & Academic Training

Lawrence Berkeley National Laboratory *Aug 2019 - Aug 2022*
Postdoc, Energy Storage and Distributed Resources Division Advisor: Prof. Kristin Persson

University of Minnesota, Twin Cities *Aug 2013 - Jul 2019*
Ph.D., Aerospace Engineering and Mechanics Advisor: Prof. Ellad Tadmor

Tianjin University *Sept 2008 - Jul 2012*
B.S., Chemical Process Machinery Engineering

Experiences

University of Houston *Sept 2022 - Present*
Assistant Professor, Department of Chemical and Biomolecular Engineering

Harvard University *Jan 2017- Jun 2017*
Visiting Student, Department of Physics

Tianjin University *Jul 2012 - Jul 2013*
Research Assistant, School of Chemical Engineering and Technology

Honors & Awards

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*

Professional Service

Reviewer for Funding Agencies

Natural Sciences and Engineering Research Council of Canada (NSERC)

Reviewer for Journals

Physical Review Letters *Physical Review B* *Physical Review Materials* *Journal of Applied Physics* *Digital Discovery* *Journal of Physics D: Applied Physics* *Machine Learning: Science and Technology* *SIAM Journal of Applied Mathematics* *2D Materials* *IOP Nanotechnology* *NeurIPS*

Publications

Preprints

2. MC Venetos, **M Wen**, and KA Persson, "Machine learning full NMR tensors with equivariant graph neural networks," *ChemRxiv,* 2022.
1. Z Shui, P Karypis, DS Karls, EB Tadmor, **M Wen**, and G Karypis, "Fine-tuning language models on multiple datasets for citation intention identification," *under review,* 2022.

Peer-reviewed papers

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,* in press, 2022.
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.

*Equal contribution

Presentations

13. Interplay between mechanics and chemistry in battery materials, *Department of Mechanics and Aerospace Engineering, Southern University of Science and Technology,* Virtual, Feb. 15, 2022 (invited).
12. Computational study of the mechanical behaviors of 2D materials, *School of Aerospace Engineering, Huazhong University of Science and Technology,* Virtual, Dec. 28, 2021 (invited).
11. Computational study of the mechanical behaviors of 2D materials, *School of Mechanical Science & Engineering, Huazhong University of Science and Technology,* Virtual, Dec. 27, 2021 (invited).

10. Computational study of the mechanical behaviors of 2D materials, *College of Science, Harbin Institute of Technology—Shenzhen,* Virtual, Dec. 10, 2021 (invited).
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

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`