

# Mingjian Wen

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## Education

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### University of Minnesota, Twin Cities

Ph.D., Aerospace Engineering and Mechanics

Sept 2013 - Jul 2019

Advisor: Prof. Ellad Tadmor

### Tianjin University

B.S., Chemical Process Machinery Engineering

Sept 2008 - Jul 2012

## Experiences

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### Lawrence Berkeley National Laboratory

Postdoc, Energy Storage and Distributed Resources Division

Aug 2019 - Present

Advisor: Prof. Kristin Persson

### Harvard University

Visiting Student, Department of Physics

Jan 2017 - Jun 2017

Advisor: Prof. Efthimios Kaxiras

### Tianjin University

Research Assistant, School of Chemical Engineering and Technology

Jul 2012 - Jul 2013

Advisor: Prof. Xu Chen

## Honors & Awards

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Doctoral Dissertation Fellowship	University of Minnesota	2018
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
National Scholarship for Graduate Students	China Ministry of Education	2012
National Scholarship for Undergraduate Students	China Ministry of Education	2010 & 2011
Outstanding Graduate from class of 2012	Tianjin University	2012

## Professional Service

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### 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*  
*IOP Nanotechnology*

## Publications

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- 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*, 2021.
- Y Kurniawan and CL Petrie and KJ Williams and MK Transtrum and EB Tadmor and RS Elliott and DS Karls and **M Wen**, Bayesian, frequentist, and information geometry approaches to parametric uncertainty quantification of classical empirical potentials, *arXiv:2112.10851*, (2021).
- 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).
- M Wen**, Y Afshar, RS Elliott, and EB Tadmor, KLIF: A framework to develop physics-based and machine learning interatomic potential, *Computer Physics Communication*, 108218 (2021).

12. 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).
11. 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).
10. **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).
9. **M Wen** and EB Tadmor, Uncertainty quantification in molecular simulations with dropout neural network potentials, *npj Computational Materials*, 6, 124 (2020).
8. **M Wen** and EB Tadmor, Hybrid neural network potential for multilayer graphene, *Physical Review B*, 100, 195419 (2019).
7. **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).
6. **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).
5. **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).
4. **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).
3. 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).
2. **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).
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.*

## Presentations

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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<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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6. KLIFF: KIM-based Learning-Integrated Fitting Framework, author, <https://kliff.readthedocs.io>
5. LAMMPS “pair\_style drip” for the DRIP Potential, author, [https://lammmps.sandia.gov/doc/pair\\_drip.html](https://lammmps.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>