Mingjian Wen

1 Cyclotron Rd, Berkeley, California 94720, USA

mjwen@berkeley.edu | https://mjwen.github.io | mjwen | mjwen

Education

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

Tianjin University — *Sep 2008 - Jul 2012*
B.S., Process Equipment and Control Engineering

Experience

University of California, Berkeley — *Aug 2019 - Present*
Postdoc, Department of Materials Science and Engineering — Advisor: Prof. Kristin Persson

Harvard University — *Jan 2017- Jun 2017*
Visiting Student, Department of Physics — Advisor: Prof. Efthimios Kaxiras

Tianjin University — *Jul 2012 - Jul 2013*
Research Assistant, School of Chemical Engineering and Technology — Advisor: Prof. Xu Chen

Honors & Awards

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*

Selected Research Projects

Graph Neural Network Model for Bond Dissociation Energy (BDE) Prediction — *Sep 2019 - Present*
- Designed a graph neural network to model charged molecules
- Designed a difference graph model to represent both homolytic and heterolytic BDEs
- Our model improves testing accuracy by 20% on a homolytic BDE dataset
- Our model achieves a testing error below the chemical accuracy for a complex BDE dataset for charged molecules

Uncertainty Quantification in Molecular simulation — *Jun 2018 - Aug 2019*
- Proposed a dropout neural network potential with the ability to quantify uncertainty in energy and forces
- Developed a powerful and practical technique to propagate the uncertainty in molecular simulation
- Applied the dropout neural network potential to study uncertainty in carbon systems

Machine Learning Potential for Multilayer Graphene — *Jun 2017 - Jan 2019*
- Developed the KLIFF package to train both physics-based and machine learning potentials
- Devised a hybrid potential for multilayer graphene that combines physical rules and machine learning techniques
- The model accurately describes both the intralayer and interlayer interactions in multilayer graphene
- Investigated friction and thermal conductivity in multilayer graphene and the effects of defects

Physics-based Registry-dependent Interlayer Potential for Graphene — *Jun 2015 - May 2017*
- Identified various problems in existing interlayer potentials
- Devised a new potential for interlayer interactions in multilayer graphene
- Computed and compared canonical properties using the potential and DFT
- Studied the peeling behavior of graphene from graphite

Skills

Computer Language	Python, C, C++, Fortran
Machine Learning Framework	PyTorch, DGL, PyTorch-Lightning, scikit-learn, TensorFlow, Keras
Simulation Code	LAMMPS, VASP, ASE, pymatgen, OpenKIM, GULP

Publications

Peer-reviewed papers

10. **M Wen**, R S Elliott, and E B Tadmor, KIM-based learning-integrated fitting framework (KLIFF), under review.
9. **M Wen**, S M Blau, E W C Spotte-Smith, S Dwaraknath and K A Persson, BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules, *Chem. Sci.,* 2021.
8. **M Wen** and E B Tadmor, Uncertainty quantification in molecular simulations with drop out neural network potentials, *npj Comput. Mater.,* 6, 124 (2020).
7. **M Wen** and E B Tadmor, Hybrid neural network potential for multilayer graphene, *Phys. Rev. B,* 100, 195419, (2019).
6. **M Wen**, S Carr, S Fang, E Kaxiras, and E B Tadmor, Dihedral-angle-corrected registry-dependent interlayer potential for multilayer graphene structures, *Phys. Rev. B,* 98, 235404 (2018).
5. **M Wen**, S N Shirodkar, P Plecháč, E Kaxiras, and E B Tadmor, A force-matching Stillinger-Weber potential for MoS_2: Parameterization and Fisher information theory based sensitivity analysis, *J. Appl. Phys.,* 122, 244301 (2017).
4. **M Wen**, J Li, P Brommer, J P Sethna, R S Elliott, and E B Tadmor, A KIM-compliant *potfit* for fitting sloppy interatomic potentials: Application to the EDIP model for silicon, *Modell. Simul. Mater. Sci. Eng.,* 25, 014001, (2017).
3. **M Wen**, S M Whalen, R S Elliott, and E B Tadmor, Interpolation effects in tabulated interatomic potentials, *Modell. Simul. Mater. Sci. Eng.,* 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, *J. Nucl. Mater.,* 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, *Mater. Des.,* 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.

Talks & Posters

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.
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.

Open-source Codes

5. LAMMPS “pair_style drip” for the DRIP Potential, contributor, https://lammps.sandia.gov/doc/pair_drip.html
4. KLIFF: KIM-based Learning-Integrated Fitting Framework, author, https://kliff.readthedocs.io
3. kimpy: a Python interface to the KIM-API, author, https://github.com/openkim/kimpy
2. BonDNet: a Graph Neural Network Model for the Prediction of Bond Dissociation Energies, author, https://github.com/mjwen/bondnet
1. Atomic Simulation Environment (ASE) KIM calculator, contributor, in collaboration with Ellad Tadmor and Dan Karls, https://wiki.fysik.dtu.dk/ase/dev/ase/calculators/kim.html