

Mingjian Wen

mjwen@lbl.gov

<https://mjwen.github.io>

Building 33, 1 Cyclotron Rd
Berkeley, California 94720, USA

EDUCATION

University of Minnesota – Twin Cities Ph.D., Aerospace Engineering and Mechanics Advisor, Professor Ellad Tadmor	Sep 2013 – Jul 2019
Tianjin University, Tianjin, China B.S., Process Equipment and Control Engineering (minor in English)	Sep 2008 – Jun 2012

EXPERIENCES

Lawrence Berkeley National Laboratory Postdoc scholar Advisor, Professor Kristin Persson	Aug 2019 – now
Department of Physics, Harvard University Visiting student Advisor, Professor Efthimios Kaxiras	Jan 2017 – Jun 2017
Department of Chemical Machinery, Tianjin University Research assistant Advisor, Professor Xu Chen	Sep 2012 – Jul 2013

HONORS & AWARDS

- *Travel Award of the Workshop on Machine Learning for Computational Fluid and Solid Dynamics*, Los Alamos National Laboratory, 2019
- *Travel Award of the Conference on Uncertainty Quantification in Computational Solid and Structural Materials Modeling*, U. S. Association for Computational Mechanics, 2019
- *Doctoral Dissertation Fellowship*, University of Minnesota, 2017 – 2018
- *National Scholarship for Graduate Students*, China Ministry of Education, 2012
- *Outstanding Graduate from class of 2012*, Tianjin University, 2012
- *National Scholarship for Undergraduate Students*, China Ministry of Education, 2010 & 2011

TECHNICAL SKILLS

Computer Languages	Python, C, C++, Fortran
Machine Learning Frameworks	PyTorch, TensorFlow, scikit-learn
Simulation Codes	LAMMPS, VASP, ASE, OpenKIM, <i>potfit</i> , GULP, SIESTA
System and Informatics	Unix, Bash, Make, L ^A T _E X, AiiDA

STUDENTS ADVISED

Neil Khadilkar	Wayzata High School	“Fracture of nanowires from DFT and interatomic potentials”
----------------	---------------------	---

SOFTWARE

1. “KIM-based Learning-Integrated Fitting Framework (KLIFF),” author. <https://kliff.readthedocs.io>.
2. “kimpy: a Python interface to the KIM-API,” author. <https://github.com/openkim/kimpy>.
3. “ASE KIM calculator,” author, in collaboration with Ellad Tadmor. <https://gitlab.com/openkim/ase>.
4. “KIM-compliant *potfit* force-matching potential fitting program,” contributor. <https://www.potfit.net>.
5. “Test Driver for linear thermal expansion coefficient of a cubic crystal,” author, https://openkim.org/cite/TD_522633393614_000.
6. “Three-body Stillinger-Weber (SW) Model Driver,” author. https://openkim.org/cite/MD_335816936951_002.

PUBLICATIONS

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. Thesis advisor: Professor Ellad Tadmor.

Papers in Refereed Journals

9. **M Wen**, R S Elliott, and E B Tadmor, “KIM-based learning-integrated fitting framework (KLIFF),” under review.
8. **M Wen** and E B Tadmor, “Uncertainty quantification in molecular simulations with dropout neural network potentials,” under review.
7. **M Wen** and E B Tadmor, “A hybrid neural network potential for multilayer graphene,” [arXiv:1909.10134](https://arxiv.org/abs/1909.10134).
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 MoS₂: 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).

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. (talk)

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. (poster)
5. “Machine learning interatomic potentials for multilayer graphene structures,” Conference on Emerging Ideas in Mechanics and Materials Science, Minneapolis, MN, Oct. 19, 2018. (talk)
4. “Interatomic potential models for 2D heterostructures,” 18th U. S. National Congress for Theoretical and Applied Mechanics (USNC/TAM), Chicago, IL, Jun. 7, 2018. (talk)
3. “Development of interatomic potentials for 2D heterostructures,” AEM Mechanics Research Seminar, University of Minnesota, Minneapolis, MN, Nov. 21, 2017. (talk)
2. “Stillinger-Weber potential for MoS₂: 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)