Contact Information

Sara Kadkhodaei
Assistant Professor
Civil and Materials Engineering
University of Illinois at Chicago, Chicago, IL 60607
e-mail: sarakad@uic.edu
website: https://cmrl.lab.uic.edu/

Education

Doctor of Philosophy, Materials Science and Engineering — May 2016
Brown University, Providence, RI
Dissertation: Free Energy Calculation of Mechanically Unstable but Dynamically Stabilized Phases
Adviser: Prof. Axel van de Walle

Master of Art, Physical Chemistry — May 2013
Brown University, Providence, RI

Bachelor of Science, Civil Engineering — June 2009
Sharif University of Technology, Tehran, Iran
Thesis: Torsional Properties of Single-walled Carbon Nanotubes
Adviser: Prof. Amir R. Khoei

Professional Experience

Assistant Professor — January 2019–present
Department of Civil, Materials, and Environmental Engineering
University of Illinois Chicago (UIC)

Postdoctoral Research Associate — June 2016– December 2018
(under the supervision of Prof. Axel van de Walle)
School of Engineering, Brown University

Current Grants

- co-PI for project "Chicago/DOE Alliance Center – A Center of Excellence for Materials at Extremes" DOE (Kadkhodaei's share: ≈$426,000/ 4 yrs), 2024-2028
- co-PI for project "Collaborative Research: DMREF: Machine Learning Algorithm Prediction and Synthesis of Next Generation Superhard Functional Materials", NSF (Kadkhodaei's share: $346,056/4 yrs), 2021-2025
- PI for project "Phonon-Assisted Diffusion in Solids from First-Principles: Unraveling a New Mechanism for Fast Diffusion.", NSF ($307,049/3 years), 2020-2024 (1-year no-cost extension)
- PI, grant for ACCESS Maximize Supercomputer Allocation of over 2M core-hours awarded in latest cycle with an estimated value of $40,028, 2023-present

Past Grants

- PI, grant for XSEDE supercomputer time allocation of over 1,500,000 core-hours/year awarded in latest cycle with an estimated value of $167,500, 2020-2022

Awards

- Outstanding Reviewer Award, Acta Journals, 2021
- College of Engineering Advising Award, UIC, 2021, 2022
- College of Engineering Research Award, UIC, 2021
- Lead Faculty of the ASM Materials Genome Toolkits Award to UIC, 2020
- Christopher B. and Susan S. Burke Civil Engineering Faculty Teaching Award, UIC, 2020
- Graduate Student Silver Award, Material Research Society (MRS), 2014
- Prager Fellowship, Brown University, 2010-2011

Teaching Experience

Courses at UIC

CME 260: Properties of Materials – undergraduate level
CME 261: Materials for Manufacturing – undergraduate level
CME 471: Thermodynamics in Materials Science – senior undergraduate level
CME 568: Kinetics of Reactions and Phase Transformations – graduate level
CME 570: Diffusion Phenomena in Materials – graduate level
CME 572: Advanced Thermodynamics in Materials Science – graduate level

Courses at Brown University

Summer School for Precollege Students: Introduction to Engineering 2014-2016

Advising Experience

Current Advisees

- Ph.D.
  - Seyyedfaridoddin Fattahpour – Ph.D. student since July 2020 – Achievements: Participated in the 2023 NSF and AFOSR sponsored workshop "Systematic Analysis of Errors and Uncertainty Across Scales from Materials Modeling & Discovery to Manufacturing: Towards Best Practices"
  - Devi Dutta Biswajeet – Ph.D. student since August 2023
  - Amir Orvati Movaffagh – Ph.D. student since August 2023
- Undergraduate
  - Connor Luttrell – Undergraduate student in my lab since January 2023

Past Advisees

- (Ph.D. (Thesis))
  - Ali Davariashtiyani – Graduated December 2023, Achievements: Participated in the 2019 NSF-sponsored University of Michigan ICME summer school, Best poster awardee at the UIC's 2021 Christopher Burke Poster Competition
- M.Sc. (Thesis)
  - Manisha M Barse - Graduated July 2023
    Thesis Title: Analysis of Defects in Ce5O9 through Density Functional Theory
- Undergraduate (Research Supervisor)

  - Caitlin Azar – Supervise 2019-2020 – Intern at QuesTek LLC during summer 2020
  - Long T. Vuong – Supervised 2020-2023, 2020 GPIP summer undergraduate intern in my lab – CURA award winner during 2020-2021 and 2021-2022, Supported by UIC's DoD-STEM 2022-2023

- Undergraduate (Thesis)
  - Noel Siony – Supported by UIC's DoD-STEM 2021-2023, 2023 UIC's Honors College Graduate in Physics, Next: Graduate Student at the University of Miami

Professional Activities/Services

- Co-organizer of the *Computational Discovery and Design of Materials* Symposium at TMS annual meeting, 2023 & 2024
- JOM Advisor, Chemistry and Physics of Materials Committee, TMS 2021-2023
- Guest editor on a special issue of the Journal of Materials (JOM): Machine Learning and New Paradigms in Computational Materials Research, Publication: September 2022
- Member of the *Chemistry and Physics of Materials* and *Alloy Phases* Commitees, TMS 2019-present
- Co-organizer of the *Computational Thermodynamics and Kinetics* Symposium at TMS annual meeting, 2020 & 2022
- Referee for *Acta Materialia*, *Physical Review Letters*, *Physical Review B*, *Physical Review Materials*, *Journal of Chemical Theory and Computation*, *Computational Materials Science*, *Scientific Reports*, *Journal of Alloys and Compounds*, *Intermetallics*, *Journal of Physics D*, *Physica Scripta*
- Grant reviewer for the National Science Foundation (NSF).
- Developer of open access software tools for the computational materials science community, including P4 software, LAMMPS local Hessian module. Supervisor for development of XIE-SPP

Invited Talks

1. "Identifying the Transition State in Structurally Unstable but Dynamically Stabilized Phases: A GPR-Assisted First Principles Methodology". In MT01: Integrating Machine Learning and Simulations for Materials Modeling. MRS Spring 2024 Meeting, Seattle, WA, April 2024
2. "Voxel image representation of crystals for accelerating inorganic materials design". In Data-driven Design of Energy Materials. ACS Fall 2023 Meeting, San Francisco, CA, August 2023
3. "How deep learning can help with materials design". In AI-Accelerated Materials Discovery II. EMRS 2023 Spring Meeting, Strasbourg – France, June 2023
4. "A new first principles approach for modeling diffusion kinetics in structurally unstable phases". In Computational Thermodynamics and Kinetics. TMS 2023 Annual Meeting, San Diego, CA, March 2023
5. "How deep learning can help with materials design". In Materials Design and Processing Optimization for Advanced Manufacturing: from Fundamentals to Application Symposium. TMS 2022 Annual Meeting, Anaheim, CA, February 2022
6. "Anharmonic lattice vibration effect on diffusion kinetics in structurally unstable phases." Computational Thermodynamics and Kinetics Symposium. TMS 2021 Virtual Meeting, USA, March 2021.
7. Understanding phase stability and diffusion kinetics of high temperature phases from first-principles, Department of Physics, University of Texas at El Paso, November 2020

8. "Understanding phase stability and diffusion kinetics in mechanically unstable but dynamically stabilized phases from first-principles", PSDK XV: Phase Stability and Diffusion Kinetics symposium, Virtual IMAT 2020, ASM's Annual Meetings, October 2020
9. Postponed: "Crystal Synthesis Prediction via Deep Learning", Materials Design, Synthesis and Manufacturing using Artificial Intelligence, 2020 International Materials Research Society Meeting, August 2020
10. "Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data", NASA Ames Research Center, Moffett Field, CA (September 06, 2018)
11. "*Ab initio* Thermodynamics and Kinetics of Materials", University of Connecticut, Storrs, CT (March 02, 2018)
12. "*Ab initio* Thermodynamics and Kinetics of Materials", University of Massachusetts at Dartmouth, North Dartmouth, MA (March 01, 2018)
13. "*Ab initio* Thermodynamics and Kinetics of Materials", University of Illinois at Chicago, Chicago, IL (February 16, 2018)
14. "Free Energy Calculation of the Mechanically Unstable but Dynamically Stabilized bcc Phase of Titanium", MRS Graduate Student Award Special Talk Session, Boston, MA (December, 2014)

Publications

GoogleScholarProfile

[1] Sara Kadkhodaei, Seyyedfaridoddin Fattahpour, and Ali Davariashtiyani. Heat radiation mitigation in rare-earth pyrosilicate composites: A first principles investigation of refractive index mismatch. *Ceramics International (Under Review)*, 2024.

[2] Seyyedfaridoddin Fattahpour and Sara Kadkhodaei. Improving ab initio diffusion calculations in materials through gaussian process regression. *Physical Review Materials (Accepted)*, 2024.

[3] Ali Davariashtiyani and Sara Kadkhodaei. Formation energy prediction of crystalline compounds using deep convolutional network learning on voxel image representation. *Communications Materials*, 4(1): 105, Dec 2023. ISSN 2662-4443. doi: 10.1038/s43246-023-00433-9. URL https://doi.org/10.1038/s43246-023-00433-9.

[4] Noel Siony, Long Vuong, Otgonsuren Lundaajamts, and Sara Kadkhodaei. Computational design of corrosion-resistant and wear-resistant titanium alloys for orthopedic implants. *Materials Today Communications*, 33:104465, 2022. ISSN 2352-4928. doi: https://doi.org/10.1016/j.mtcomm.2022.104465. URL https://www.sciencedirect.com/science/article/pii/S235249282201306X.

[5] Vanessa Meraz, Sofia Gomez, Valeria Arteaga Muniz, Adrian De la Rocha Galán, Tess Smidt, Sara Kadkhodaei, Wibe de Jong, and Jorge Munoz. Zirconium machine learned potential trained on a euclidean neural network. *Bulletin of the American Physical Society*, 2022.

[6] Seyyedfaridoddin Fattahpour, Ali Davariashtiyani, and Sara Kadkhodaei. Understanding the role of anharmonic phonons in diffusion of bcc metals. *Phys. Rev. Materials*, 6:023803, Feb 2022. doi: 10.1103/PhysRevMaterials.6.023803. URL https://link.aps.org/doi/10.1103/PhysRevMaterials.6.023803.

[7] Ali Davariashtiyani, Zahra Kadkhodaie, and Sara Kadkhodaei. Predicting synthesizability of crystalline materials via deep learning. *Communications Materials*, 2(1):115, Nov 2021. ISSN 2662-4443. doi: 10.1038/s43246-021-00219-x. URL https://doi.org/10.1038/s43246-021-00219-x.

[8] Sara Kadkhodaei and Jorge A. Muñoz. Cluster expansion of alloy theory: A review of historical development and modern innovations. *JOM*, Sep 2021. ISSN 1543-1851. doi: 10.1007/s11837-021-04840-6. URL https://doi.org/10.1007/s11837-021-04840-6.

[9] Sara Kadkhodaei and Ali Davariashtiyani. Phonon-assisted diffusion in bcc phase of titanium and zirconium from first principles. *Phys. Rev. Materials*, 4:043802, Apr 2020. doi: 10.1103/PhysRevMaterials.4.043802. URL https://link.aps.org/doi/10.1103/PhysRevMaterials.4.043802.

[10] Sara Kadkhodaei and Axel van de Walle. Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data. *Computer Physics Communications*, 246:106712, 2020. ISSN 0010-4655. doi: https://doi.org/10.1016/j.cpc.2019.01.008. URL http://www.sciencedirect.com/science/article/pii/S0010465519300141.

[11] Sara Kadkhodaei and A. van de Walle. A simple local expression for the prefactor in transition state theory. *The Journal of Chemical Physics*, 150(14):144105, 2019. doi: 10.1063/1.5086746. URL https://doi.org/10.1063/1.5086746.

[12] Sara Kadkhodaei and Axel van de Walle. First-principles calculations of thermal properties of the mechanically unstable phases of the PtTi and NiTi shape memory alloys. *Acta Materialia*, 147:296 – 303, 2018. ISSN 1359-6454. doi: https://doi.org/10.1016/j.actamat.2018.01.025. URL http://www.sciencedirect.com/science/article/pii/S1359645418300569.

[13] Axel van de Walle, Sara Kadkhodaei, Ruoshi Sun, and Qi-Jun Hong. Epicycle method for elasticity limit calculations. *Phys. Rev. B*, 95:144113, Apr 2017. doi: 10.1103/PhysRevB.95.144113. URL https://link.aps.org/doi/10.1103/PhysRevB.95.144113.

[14] Sara Kadkhodaei, Qi-Jun Hong, and Axel van de Walle. Free energy calculation of mechanically unstable but dynamically stabilized bcc titanium. *Phys. Rev. B*, 95:064101, Feb 2017. doi: 10.1103/PhysRevB.95.064101. URL https://link.aps.org/doi/10.1103/PhysRevB.95.064101.

[15] Axel van de Walle, Ruoshi Sun, Qi-Jun Hong, and Sara Kadkhodaei. Software tools for high-throughput calphad from first-principles data. *Calphad*, 58(Supplement C):70 – 81, 2017. ISSN 0364-5916. doi: https://doi.org/10.1016/j.calphad.2017.05.005. URL http://www.sciencedirect.com/science/article/pii/S0364591617300305.

[16] Axel van de Walle, Qijun Hong, Sara Kadkhodaei, and Ruoshi Sun. The free energy of mechanically unstable phases. *Nature Communications*, 6:7559, 2015. URL https://doi.org/10.1038/ncomms8559.

[17] Teng Zhang, Xiaoyan Li, Sara Kadkhodaei, and Huajian Gao. Flaw insensitive fracture in nanocrystalline graphene. *Nano Letters*, 12(9):4605–4610, 2012. doi: 10.1021/nl301908b. URL http://dx.doi.org/10.1021/nl301908b.