Sara Kadkhodaei
Assistant Professor
University of Illinois Chicago
Civil, Materials, and Environmental Engineering
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Education

Ph.D. in Science Engineering, Brown University 2016
Dissertation: Free Energy Calculation of Mechanically Unstable but Dynamically Stabilized Phases
Adviser: Prof. Axel van de Walle

M.A. in Physical Chemistry, Brown University 2013

B.Sc. in Civil Engineering (Summa cum laude), Sharif University of Technology 2009

Appointments

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

Postdoctoral Research Associate (with Prof. van de Walle), Brown University 2016–2018
School of Engineering

Current Grants

- co-PI for the project "Chicago/DOE Alliance Center – A Center of Excellence for Materials at Extremes" DOE-NNSA (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, grant for ACCESS Maximize Supercomputer Allocation of over 2M core-hours awarded in latest cycle with an estimated value of $72,400, 2023-present

Past Grants

- 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 XSEDE supercomputer time allocation of over 1,500,000 core-hours/year awarded in latest cycle with an estimated value of $177,890, 2020-2022

Awards

- College of Engineering Teaching Award, UIC, 2024
- 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, 2023
- 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

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

Advising

Current Graduate Students (PhD): Devi Dutta Biswajeet (2023-), Amir Orvati Movaffagh (2023-), Seyyedfaridoddin Fattahpour (2020-)

Former Graduate Students (PhD): Ali Davariashtiyani (PhD, 2019-2023, Now at the University of Chicago), Manisha Barse (MS, 2022-2023, Now at Leiber Institute for Brain Development)

Undergraduate Students Supervised (most recent first): Caleb Williams (Electrical Eng. & Physics, 2023-), Saleha Hashima (Chemical Eng., 2023-), Moiz Zafar Shakir (Mechanical Eng., 2023-), Jakub Mitka (UIUC Mechanical Eng., 2023), Connor Luttrell (Electrical Eng., 2022-), Noel Siony (Physics, 2021-2023), Otgonsuren Lundaajamts (Mechanical Eng., 2021-2022), Long T. Vuong (Mechanical Eng., 2020-2023), Caitlin Azar (Mechanical Eng., 2019-2020)

Service

- Member of the *Content Development & Dissemination Committee*, TMS (2025-present)
- Co-organizer of the *Integrating Machine Learning and Simulations for Materials Modeling* Symposium, MRS Fall 2025 Meeting (Upcoming – December 2025)
- Co-organizer of the *Computational Discovery and Design of Materials* Symposium, TMS 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, TMS meeting (2020 & 2022)
- Referee for *The Journal of Chemical Physics*, *Crystal Growth & Design* , *Chemistry of Materials* , *Journal of Applied Physics* , *npj Computational Materials*, *Journal of Materials Science*, *CALPHAD*, *Physical Review Research*, *Scientific Reports*, *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*, *Scripta Materialia*
- Proposal reviewer for the National Science Foundation (NSF) and Department of Energy (DOE).
- 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. "Enhancing insight and design of future materials through theoretical modeling and artificial intelligence", Materialize the Future Workshop, Master of Materiomics program, Hasselt University, April 2024 (Online)
3. "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
4. "How deep learning can help with materials design". In AI-Accelerated Materials Discovery II. EMRS 2023 Spring Meeting, Strasbourg – France, June 2023
5. "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
6. "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
7. "Anharmonic lattice vibration effect on diffusion kinetics in structurally unstable phases." Computational Thermodynamics and Kinetics Symposium. TMS 2021 Virtual Meeting, USA, March 2021.
8. Understanding phase stability and diffusion kinetics of high-temperature phases from first-principles, Department of Physics, University of Texas at El Paso, November 2020
9. "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
10. Postponed: "Crystal Synthesis Prediction via Deep Learning", Materials Design, Synthesis and Manufacturing using Artificial Intelligence, 2020 International Materials Research Society Meeting, August 2020
11. "Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data", NASA Ames Research Center, Moffett Field, CA (September 06, 2018)
12. "*Ab initio* Thermodynamics and Kinetics of Materials", University of Connecticut, Storrs, CT (March 02, 2018)
13. "*Ab initio* Thermodynamics and Kinetics of Materials", University of Massachusetts at Dartmouth, North Dartmouth, MA (March 01, 2018)
14. "*Ab initio* Thermodynamics and Kinetics of Materials", University of Illinois at Chicago, Chicago, IL (February 16, 2018)
15. "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] Pardis Seraji, Hessam Shahbazi, Musawenkosi K. Ncube, Nannan Shan, Francisco Lagunas, Ilias Papailias, Pouyan Navabi, Chengji Zhang, Ahmad Jaradat, Sara Kadkhodaei, Ksenija D. Glusac, Robert F. Klie, Anh T. Ngo, Larry A. Curtiss, and Amin Salehi-Khojin. "Stabilizing lithium superoxide formation in lithium-air batteries by Janus chalcogenide catalysts". In: *Nano Energy* 134 (2025), p. 110510. ISSN: 2211-2855. DOI: https://doi.org/10.1016/j.nanoen.2024.110510. URL: https://www.sciencedirect.com/science/article/pii/S221128552401262X.

[2] Ali Davariashtiyani, Busheng Wang, Samad Hajinazar, Eva Zurek, and Sara Kadkhodaei. "Impact of data bias on machine learning for crystal compound synthesizability predictions". In: *Machine Learning: Science and Technology* 5.4 (2024), p. 040501. DOI: 10.1088/2632-2153/ad9378. URL: https://dx.doi.org/10.1088/2632-2153/ad9378.

[3] Amir M. Orvati Movaffagh, Adetoye Adekoya, and Sara Kadkhodaei. "Defect energy formalism for CALPHAD thermodynamics of dilute point defects". In: *Phys. Rev. Mater.* 8 (11 2024), p. 113802. DOI: 10.1103/PhysRevMaterials.8.113802. URL: https://link.aps.org/doi/10.1103/PhysRevMaterials.8.113802.

[4] Hessam Shahbazi, Pardis Seraji, Husam Faraj, Taimin Yang, Allen Kim, Seyyedfaridoddin Fattahpour, Ilias Papailias, Matthew Diamond, Shahriar Namvar, Alireza Ahmadiparidari, Shuxi Wang, Zhenxian Liu, Khahesh Kumar, Muhetaer Aihaiti, Jordi Cabana, Sara Kadkhodaei, Junlan Wang, Zhehao Huang, Russell J. Hemley, and Amin Salehi-khojin. Resiliency, Morphology, and Transformations of a One-Dimensional High-Entropy Oxide. Science (Revision Submitted). 2024.

[5] Sara Kadkhodaei, Seyyedfaridoddin Fattahpour, and Ali Davariashtiyani. "Heat radiation mitigation in rare-earth pyrosilicate composites: A first principles investigation of refractive index mismatch". In: *Ceramics International* 50.9, Part A (2024), pp. 15021–15036. DOI: https://doi.org/10.1016/j.ceramint.2024.01.417. URL: https://www.sciencedirect.com/science/article/pii/S0272884224004449.

[6] Seyyedfaridoddin Fattahpour and Sara Kadkhodaei. "Improving ab initio diffusion calculations in materials through Gaussian process regression". In: *Phys. Rev. Mater.* 8 (1 2024), p. 013804. DOI: 10.1103/PhysRevMaterials.8.013804. URL: https://link.aps.org/doi/10.1103/PhysRevMaterials.8.013804.

[7] Ali Davariashtiyani and Sara Kadkhodaei. "Formation energy prediction of crystalline compounds using deep convolutional network learning on voxel image representation". In: *Communications Materials* 4.1 (2023), p. 105. ISSN: 2662-4443. DOI: 10.1038/s43246-023-00433-9. URL: https://doi.org/10.1038/s43246-023-00433-9.

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

[9] 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". In: *Bulletin of the American Physical Society* (2022).

[10] Seyyedfaridoddin Fattahpour, Ali Davariashtiyani, and Sara Kadkhodaei. "Understanding the role of anharmonic phonons in diffusion of bcc metals". In: *Phys. Rev. Materials* 6 (2 2022), p. 023803. DOI: 10.1103/PhysRevMaterials.6.023803. URL: https://link.aps.org/doi/10.1103/PhysRevMaterials.6.023803.

[11] Ali Davariashtiyani, Zahra Kadkhodaie, and Sara Kadkhodaei. "Predicting synthesizability of crystalline materials via deep learning". In: *Communications Materials* 2.1 (2021), p. 115. ISSN: 2662-4443. DOI: 10.1038/s43246-021-00219-x. URL: https://doi.org/10.1038/s43246-021-00219-x.

[12] Ali Davariashtiyani. XIE-SPP: Crystal Image Encoder for Synthesis & Property Prediction. https://github.com/kadkhodaei-research-group/XIE-SPP. 2021.

[13] Sara Kadkhodaei and Jorge A. Muñoz. "Cluster Expansion of Alloy Theory: A Review of Historical Development and Modern Innovations". In: *JOM* (2021). ISSN: 1543-1851. DOI: 10.1007/s11837-021-04840-6. URL: https://doi.org/10.1007/s11837-021-04840-6.

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

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

[16] Sara Kadkhodaei and A. van de Walle. "A simple local expression for the prefactor in transition state theory". In: *The Journal of Chemical Physics* 150.14 (2019), p. 144105. DOI: 10.1063/1.5086746. eprint: https://doi.org/10.1063/1.5086746. URL: https://doi.org/10.1063/1.5086746.

[17] Sara Kadkhodaei. Piecewise Polynomial Potential Partitioning (P4) Software. https://sarakad.github.io/P4/. 2019.

[18] Sara Kadkhodaei. LAMMPS Local Hessian. https://sarakad.github.io/lammps_local_hessian/. 2019.

[19] 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". In: *Acta Materialia* 147 (2018), pp. 296 –303. ISSN: 1359-6454. DOI: https://doi.org/10.1016/j.actamat.2018.01.025. URL: http://www.sciencedirect.com/science/article/pii/S1359645418300569.

[20] Axel van de Walle, Sara Kadkhodaei, Ruoshi Sun, and Qi-Jun Hong. "Epicycle method for elasticity limit calculations". In: *Phys. Rev. B* 95 (14 2017), p. 144113. DOI: 10.1103/PhysRevB.95.144113. URL: https://link.aps.org/doi/10.1103/PhysRevB.95.144113.

[21] Sara Kadkhodaei, Qi-Jun Hong, and Axel van de Walle. "Free energy calculation of mechanically unstable but dynamically stabilized bcc titanium". In: *Phys. Rev. B* 95 (6 2017), p. 064101. DOI: 10.1103/PhysRevB.95.064101. URL: https://link.aps.org/doi/10.1103/PhysRevB.95.064101.

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

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

[24] Teng Zhang, Xiaoyan Li, Sara Kadkhodaei, and Huajian Gao. "Flaw Insensitive Fracture in Nanocrystalline Graphene". In: *Nano Letters* 12.9 (2012), pp. 4605–4610. DOI: 10.1021/nl301908b. eprint: http://dx.doi.org/10.1021/nl301908b. URL: http://dx.doi.org/10.1021/nl301908b.