Curriculum Vitae

Siya Zhu, Ph.D.

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Computational materials scientist specializing in thermodynamics and atomistic simulations, including first-principles calculations, molecular dynamics, Monte Carlo simulations, and machine learning–driven materials discovery. Investigates phase stability, phase diagram calculations, metallic glass, defect and impurity behavior in complex and high-entropy alloy systems.

Professional Experience

Jun. 2024 – **Postdoctoral Researcher** Texas A&M University.
Computational materials research focusing on alloy thermodynamics and phase diagram calculations with machine-learning potentials, mechanical stability of alloys, and interstitial in high-entropy alloys.

Jun. 2023 – May 2024 **Postdoctoral Researcher** Brown University.
Research on CALPHAD modeling and alloy phase diagram computations; Atomic structures and mechanical properties of bulk metallic glasses.

Jun. 2021 – Dec. 2021 **Student Intern** Lawrence Livermore National Laboratory.
Theoretical research on Orbital-free Density Functional Theories; Research on high-entropy alloys with the cluster expansion modeling

Education

Sept. 2016 – May. 2023 **Ph.D., Brown University** Material Science and Engineering

Sept. 2012 – Jun. 2016 **Bachelor, Peking University** Material Science and Engineering

Research Software Developed

MAST **Metallic Amorphous Structures Toolkit** — *Developed and maintained* research software framework for generating Special Glass Structures (SGS) that reproduce target structural descriptors, enabling large-scale simulations of amorphous networks. Open-source: `https://github.com/siyazhu/MAST`

PhaseForge **PhaseForge** — *Co-developed* a framework for high-throughput alloy phase diagram prediction using machine-learning interatomic potentials (MLIPs) integrated with ATAT and CALPHAD modeling, with primary responsibility for algorithm design, workflow implementation, core code development and validation. Open-source: `https://github.com/dogusariturk/PhaseForge`

PhaseForge+ **PhaseForgePlus** — *Co-developed* a framework for generating and tuning physically-informed CALPHAD models, upon the foundation of PhaseForge, with responsibility for coding, data analysis and validation. Open-source: `https://github.com/dogusariturk/PhaseForgePlus`

Research Software Developed (continued)

PAIPAI — **Package for Alloy Interstitial Predictions using Artificial Intelligence** — *Developed and maintained* a computational tool for efficient exploration of low-free-energy metallic structures containing interstitials and defects, using Monte Carlo sampling and machine-learning interatomic potentials. Open-source: `https://github.com/siyazhu/PAIPAI`

Publication List

First-author publications

1. **Zhu, S.** and Arróyave, R., 2026. "Ground-state structure search of defective high-entropy alloys using machine-learning potentials and Monte Carlo sampling." *Computational Materials Science*, 270, p.114752.
2. **Zhu, S.**, Eckert, H., Curtarolo, S., Schroers, J. and van de Walle, A., 2026. "Computational Study of Density Fluctuation-Facilitated Shear Bands Formation in Bulk Metallic Glasses." *npj Computational Materials* 12, 157.
3. **Zhu, S.**, Sarıtürk, D. and Arróyave, R., 2025. "Accelerating CALPHAD-based phase diagram predictions in complex alloys using universal machine learning potentials: Opportunities and challenges." *Acta Materialia*, 286, p.120747.
4. **Zhu, S.**, Sarítürk, D. and Arróyave, R., 2025. "Machine learning potentials for alloys: a detailed workflow to predict phase diagrams and benchmark accuracy." *npj Computational Materials*, 11(1), p.340.
5. **Zhu, S.**, Schroers, J., Curtarolo, S., Eckert, H. and van de Walle, A., 2024. "Special glass structures for first principles studies of bulk metallic glasses." *Acta Materialia*, 262, p.119456.
6. **Zhu, S.**, Shittu, J., Perron, A., Nataraj, C., Berry, J., McKeown, J.T., van de Walle, A. and Samanta, A., 2023. "Probing phase stability in CrMoNbV using cluster expansion method, CALPHAD calculations and experiments." *Acta Materialia*, 255, p.119062.
7. **Zhu, S.** and van de Walle, A., 2021. "Computational Assessment of Novel Predicted Compounds in Ni-Re Alloy System." *Journal of Phase Equilibria and Diffusion*, 42(2), pp.315-320.
8. **Zhu, S.** and Wang, Q., 2015. "A simple method for understanding the triangular growth patterns of transition metal dichalcogenide sheets." *AIP Advances*, 5(10).

Manuscripts under review

1. **Zhu, S.** and Arróyave, R., 2026. "Influence of Coherent Elastic Strain on Phase Separation in BCC Nb-V Alloys." *submitted to Acta Materialia, arXiv preprint arXiv:2605.01031.*
2. Tavakolzadeh, M., Sheu, E., Motallebi, R., **Zhu, S.**, Arróyave, R., Xie, K., and Demkowicz, M., 2026. "Thermodynamically metastable Cu-V solid solution enabled by pseudomorphism." *submitted to Nano Letters*.

Other Publications

1. Yan, K., Bohde, M., Kryvenko, A., Xiang, Z., Zhao, K., **Zhu, S.**, Kolachina, S., Sarıtürk, D., Xie, J., Arróyave, R., Qian, X., Qian, X. and Ji, S., 2026. "Learning Materials Interatomic Potentials via Hybrid Invariant-Equivariant Architectures." *Accepted by Transactions on Machine Learning Research (TMLR). Available on OpenReview: https://openreview.net/forum?id=fq3nrVqNmL*
2. Huang, A., **Zhu, S.**, Belcher, C., Rigsby, R., Apelian, D., Arróyave, R. and Lavernia, E.J., 2026. "Predicting Interstitial Solutes in Refractory Complex Concentrated Alloys via a Combined Experimental and Computational Workflow: A Case Study on Oxygen in NbTaTiHf." *Acta Materialia*, 308, p.122019.
3. Kunselman, C., **Zhu, S.**, Sarıtürk, D. and Arróyave, R., 2025. "Construction and Tuning of CALPHAD Models Using Machine-Learned Interatomic Potentials and Experimental Data: A Case Study of the Pt–W System." *Journal of Phase Equilibria and Diffusion*, pp.1-9.

4. Eckert, H., Kube, S.A., Divilov, S., Guest, A., Zettel, A.C., Hicks, D., Griesemer, S.D., Hotz, N., Campilongo, X., **Zhu, S.** and van de Walle, A., 2025. "Soliquidy: a descriptor for atomic geometrical confusion." *npj Computational Materials*, 11(1), p.40.
5. Chen, H., Samanta, S., **Zhu, S.**, Eckert, H., Schroers, J., Curtarolo, S. and van de Walle, A., 2024. "Bayesian active machine learning for Cluster expansion construction." *Computational Materials Science*, 231, p.112571.
6. van de Walle, A., Samanta, S., Nataraj, C., **Zhu, S.**, Chen, H., Liu, H. and Arroyave, R., 2023. "Revisiting the SGTE lattice stability of bcc aluminum." *Calphad*, 83, p.102628.
7. Kumar, S., Borda, E.L., Sadigh, B., **Zhu, S.**, Hamel, S., Gallagher, B., Bulatov, V., Klepeis, J. and Samanta, A., 2022. "Accurate parameterization of the kinetic energy functional." *The Journal of Chemical Physics*, 156(2).
8. Kumar, S., Sadigh, B., **Zhu, S.**, Suryanarayana, P., Hamel, S., Gallagher, B., Bulatov, V., Klepeis, J. and Samanta, A., 2022. "Accurate parameterization of the kinetic energy functional for calculations using exact-exchange." *The Journal of Chemical Physics*, 156(2).
9. van de Walle, A., Chen, H., Liu, H., Nataraj, C., Samanta, S., **Zhu, S.** and Arroyave, R., 2022. "Interactive exploration of high-dimensional phase diagrams." *JOM*, 74(9), pp.3478-3486.
10. Fang, Q., Zhang, Z., Ji, Q., **Zhu, S.**, Gong, Y., Zhang, Y., Shi, J., Zhou, X., Gu, L., Wang, Q. and Zhang, Y., 2017. "Transformation of monolayer MoS2 into multiphasic MoTe2: Chalcogen atom-exchange synthesis route." *Nano Research*, 10(8), pp.2761-2771.
11. Jia, B., Wu, Y., Zhao, F., Yan, C., **Zhu, S.**, Cheng, P., Mai, J., Lau, T.K., Lu, X., Su, C.J. and Wang, C., 2017. "Rhodanine flanked indacenodithiophene as non-fullerene acceptor for efficient polymer solar cells." *Science China Chemistry*, 60(2), pp.257-263.
12. Wu, Y., Bai, H., Wang, Z., Cheng, P., **Zhu, S.**, Wang, Y., Ma, W. and Zhan, X., 2015. "A planar electron acceptor for efficient polymer solar cells." *Energy and Environmental Science*, 8(11), pp.3215-3221.

Skills

Languages	Mandarin Chinese, English.
Coding	Java, C, C++, MATLAB, Python, LaTeX
Computational Software	VASP, LAMMPS

Conferences

2026
- **Zhu, S.**, Sarıtürk, D., Arróyave, R., "PhaseForge: A Framework for Phase Diagram Predictions and Benchmarking Using Machine Learning Potentials". 2026 TMS Annual Meeting & Exhibition, 03/17/2026.

2024
- **Zhu, S.**, Samanta, A., Shittu, J., Perron A., Nataraj, C., Berry, J., Mckeown, J., van de Walle, A., "Probing Phase Stability in CrMoNbV Using Cluster Expansion Method, Calphad Calculations and Experiments". 2024 MRS Fall Meeting, Boston, 12/03/2024
- **Zhu, S.**, Eckert, H., Curtarolo, S., Schroers, J., van de Walle, A., "Unveiling the Formation of Shear Bands in Metallic Glass — A Hypothesis on the Influence of Low-Density Regions and Density Fluctuations". 2024 MRS Fall Meeting, Boston, 12/03/2024

2023
- **Zhu, S.**, Schroers, J., Curtarolo, S., Eckert, H., van de Walle, A., "Special glass structures for first principles studies of bulk metallic glasses". 2023 MRS Fall Meeting, Boston, 11/27/2023

2020
- **Zhu, S.**, van de Walle, A. “Towards High-Throughput First-Principles High-Temperature Thermodynamic Modeling”. 2020 MRS Fall Meeting, virtual, 12/04/2020.