



## Changzhi Ai

Postdoctoral Scholar, Photon Science, SLAC

### Bio

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#### BIO

Changzhi Ai is a Postdoctoral Researcher at the SUNCAT Center for Interface Science and Catalysis at Stanford University and SLAC National Accelerator Laboratory. He specializes in developing machine learning models for surface and interfacial chemistry, with broader expertise in atomistic modeling for materials science and chemistry. His research also explores agentic AI for scientific discovery, automation of active learning workflows, global optimization algorithms, and high-throughput materials screening. He obtained his PhD from the Technical University of Denmark.

His current research focuses on the development of scalable, physically informed machine learning potentials, particularly equivariant neural network architectures, for accurately modeling complex chemical environments. His work spans heterogeneous catalysis, multi-metallic alloy design, reaction kinetics, and surface and interfacial chemistry, with an emphasis on uncovering structure–property relationships at the atomic scale.

In addition, he has extensive experience integrating machine learning models into simulation pipelines and deploying them in large-scale computational environments. His technical expertise includes deep learning frameworks such as PyTorch, distributed training (DDP and multi-node GPU systems), and scientific computing tools including LAMMPS, ASE, and TorchScript/LibTorch for production-level deployment. He also develops end-to-end automated workflows for data generation, model training, and adaptive sampling in materials discovery.

#### Keywords:

Machine Learning Potentials (Equivariant GNNs), Atomistic Simulations, Molecular Dynamics, Active Learning & Workflow Automation, High-Throughput Screening, Global Optimization Algorithms, Scientific Machine Learning, Distributed GPU Computing, PyTorch & TorchScript, LAMMPS Integration, ASE, HPC Systems, Data-Driven Materials Discovery

#### Code & Projects:

GitHub: <https://github.com/changzhiai>

#### PROFESSIONAL EDUCATION

- Doctor of Philosophy, Technical University of Denmark Biosustain BRIGHT (2023)
- PhD, Technical University of Denmark (2023)

#### STANFORD ADVISORS

- Dimosthenis Sokaras, Postdoctoral Research Mentor
- Britt Hedman, Postdoctoral Faculty Sponsor