Xinzhe Dai

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EDUCATION

University of Chinese Academy of Sciences (UCAS) Beijing
B.S. Candidate, School of Physical Sciences (GPA: 3.85) Sep. 2019 - Jun. 2024
Core Courses: Computational Materials Science, Introduction to Computational Chemistry, Group Theory, Introduction to Solid State Physics

RESEARCH EXPERIENCE

Visiting Student, *Department of Material Sci. & Eng.* **UCB** Jun. 2023 – May. 2024
Advisor: Prof. Gerbrand Ceder
Research Project: *Universal Interatomic Potential: Benchmarked with NequIP*

- Investigated the influence of data size and symmetry on machine learning universal interatomic potential.
- Explored the tricks to improve the universal potential performance.

Research Project: *Universal Material Generation with Diffusion (CHGGEN)*

- Adapted a Variational Autoencoder (VAE)-based model and pre-trained CHGNet for more efficient crystal structure representation.
- Implemented a score-based diffusion model for stable material generation.
- Conducted property-guided material generation to create materials with specific desired properties.

Research Intern*, School of Physical Sciences*, **UCAS** Oct. 2021 – Aug. 2024
Advisor: Prof. Wu Zhou
Research Project: *DeepSTEM: Copilot for STEM Z-contrast Imaging and STEM-EELS Data Processing and Analysis*

- High-precision chemical characterization with STEM
- Structural analysis and physical properties of amorphous monolayer carbon: r-VAE
- Isotope mapping at atomic resolution: EELS denoising with statistical learning
- Details can be found here.

Related Publication: Low-dose imaging denoise with one pair of noise images. *Optics Express* (2023) Yang, D., Lv, W., Zhang, J., Chen, H., Sun, X., Lv, S., **Dai, X.**, Luo, R., Zhou, W., Shi, Y., Qiu, J.

Research Intern*, Department of Material Sci. & Eng.* **MIT** May. 2022 – Jul. 2022
Advisor: Prof. Rodrigo Freitas
Research Project: *Data-centric Crystal Structure Identification in Atomistic Simulations*

- Used graph convolution neural network as a classifier to identify local crystal structure in simulations, reducing the error rate by 2-5 times for different structures.
- Used feature engineering to reduce the computational cost by about 3 times, narrowing the gap of time cost between our algorithm and heuristic algorithms.

Research Intern*, School of Physical Sciences*, **UCAS** Mar. 2021 - Oct. 2021

Advisor: Prof. Qian Liu
Research Project: *Reconstruction Algorithm in Cosmic Ray Muon Imaging*

- Reconstructed the composition and shape of block material with scattering imaging.
- Explored the applicability and performance of the algorithm with Geant4 simulation data.

Research Project: *Neutron and Gamma Ray Shape Discrimination with Machine Learning*

- Discriminated neutron and gamma ray with 99.85% accuracy using 9-layer CNN.
- Showed the effectiveness of this method with similar performance as traditional method.

TEACHING EXPERIENCE

***Teaching Assistant**, School of Physical Sciences,* **UCAS** Sep. 2022 - Dec. 2022
Lecture: Undergraduate Thermodynamics and Statistical Physics (Taught in English)

- The topics include phase transition, ensemble theory, quantum statistics, etc.

HONORS AND AWARDS

University of Chinese Academy of Sciences (UCAS)
Academic Scholarship Oct. 2022, 2021, 2020

University of Chinese Academy of Sciences (UCAS)
Overseas Graduate Studies Fellowship Sep. 2022

EXTRACURRICULAR ACTIVITIES

AI + Science Academic Platform
Initiator/ Cross-Disciplinary and Open Discussion Platform on AI + Sci. Mar. 2023 – Jun. 2023

DeepSTEM @ UCAS
Leader/ Group Implementing AI Tools in Electron Microscopy Apr. 2023 - Jun. 2023

NetEase Cloud Music
Campus Songwriter/ Popular Music and Light Music Aug. 2021 – Jun. 2023

Public Welfare Education Service Center Changsha
Volunteer/Online Tutor for Senior High School Math and Physics May. 2020 - Aug. 2020

SKILLS

TOEFL:104 (R29, L27, S23, W25) Jul. 2022
GRE: 323 (V155, Q168, W3.0) Jun. 2022
Proficient in Python, Pytorch, Origin, Material Studio (CASTEP), Gaussian
Frequent user of Shell, Ovito, C, LAMMPS
Familiar with C++, MATLAB

REFERENCES

Prof. Gerbrand Ceder (gceder@berkeley.edu)
University of California, Berkeley

Prof. Wu Zhou (wuzhou@ucas.ac.cn)
University of Chinese Academy of Sciences