

Qifan Yang

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🎓 Education

- › **Huazhong University of Science and Technology(HUST), Wuhan, China** Aug 2023 - Present
M.Sc. in Materials Science and Engineering Research Advisor: Prof. Tianyou Zhai and Dr. Yinghe Zhao
Courses: Multiscale simulation of materials, Fundamentals of Materials Chemistry, Advanced solid state physics, Machine Learning.
- › **Huazhong University of Science and Technology(HUST), Wuhan, China** Aug 2019 - Jun 2023
B.Eng. in Materials Science and Engineering GPA:3.81/4.00
Selected Courses: Quantum Mechanics, Materials Physics, Physical Chemistry, Computational Materials Science, Fundamentals of Materials Science, Introduction to Artificial Intelligence.

leftrightarrow Research Experience

- #1. **Quantum Embedding Framework for ORR Mechanism on Fe-N-C Catalysts** Apr 2024 - Oct 2025
› Developed a periodic quantum embedding framework based on Density Matrix Embedding Theory (DMET) to perform CCSD(T)-level energy calculations for Fe-N-C single-atom catalysts. [Code]
- › Calibrated DFT functionals with CCSD(T) benchmarks, identifying the RPBE functional as the most reliable for Fe-N-C ORR energetics.
- › Applied the RPBE functional to periodic bulk Fe-N₄ models, revealing intrinsically high ORR activity.
- #2. **EGNN for Synthesizability Prediction of Two-Dimensional(2D) Materials** Nov 2023 - Feb 2024
› Collected and curated 6,399 2D crystal structures from the C2DB and MC2D databases for synthesizability classification using an Equivariant Graph Neural Network (EGNN).
› Achieved superior performance over CGCNN across multiple evaluation metrics, attaining an accuracy of 94.35 %.
- #3. **High-Throughput Screening of Two-Dimensional(2D) Ferroelectrics** Nov 2022 - Apr 2023
› Built a high-throughput screening framework, integrating C2DB and MC2D databases for 2D materials discovery.
› Designed stability and symmetry-based descriptors to filter potential out-of-plane ferroelectric materials.

📄 Manuscript

- › **Qifan Yang, Yinghe Zhao, Tianyou Zhai.** Is the basal plane of bulk Fe-N-C materials really inactive for the oxygen reduction reaction?. In preparation.

🔧 Skills

- › *Programming* Python, Markdown, LaTeX, Bash, Linux HPC
› *Data Analysis Tools* PyTorch, Numpy, Scikit-learn, Pandas, Matplotlib
› *Computational Material Tools* VASP, PySCF, VESTA, Materials Studio

🎖 Honors and Awards

- › *First-Class Academic Scholarship* , HUST Oct 2023
› *Outstanding Graduate Award* , HUST Jun 2019

👤 Academic Service

- › Teaching Assistant, *Computational Materials Science (Fall 2018)*, HUST