Qifan Yang

https://xp1037.github.io/ @ yqf_@hust.edu.cn (+86) 17607114907

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 Assoc. Prof. 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 WGPA: 3.91/4.00
  Selected Courses: Data Structures and Algorithm Analysis (100), Linear Algebra (100), Introduction to Computer Programming (98), Artificial Intelligence (96), Probability and Statistics (96).

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. [Project]
- 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-N_4 models, revealing intrinsically high ORR activity.

#2. Equivariant Graph Neural Network 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.

Publications

- Zhehan Kan, Shuoshuo Chen, **Qifan Yang**, Yushun Tang, *et al.* Self-Correctable and Adaptable Inference for Generalizable Human Pose Estimation. In *IEEE/CVF Conference on Computer Vision and Pattern Recognition* (*CVPR*), 2023. [PDF]

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

 Last Edited: 2025.10.30