




# 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.

## 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-N<sub>4</sub> 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