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 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_4 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.

#4. Computational Support for Experimental Materials Research *Nov 2023 - Oct 2025*

- Conducted DFT-based calculations to investigate ion and molecule migration mechanisms in low-dimensional and molecular materials(e.g.,$MoSi_2N_4$, $C_{60} \cdot 2P_4Se_3$), including migration barrier evaluation via NEB methods.
- Systematically analyzed the impact of structural motifs and vacancy configurations on migration barriers, providing mechanistic understanding for experimentally observed transport behaviors.
- Performed optical property calculations (dielectric function, optical transitions) for anisotropic 2D materials (e.g., ReS_2), supporting interpretation of polarization-dependent optical experiments.

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

 Last Edited: 2025.12.17