JIAWEI CHEN

Crystal Structure Prediction (CSP) / Machine Learning (ML) / First-Principles Calculations

2285450581@qq.com github.com/chen121760
Guangdong University of Technology
M.S. in Materials Physics and Chemistry
Guangzhou, Guangdong, China

Skills

Programming Python, Bash, LaTeX
Software & Tools VASP, Quantum ESPRESSO, USPEX, SISSO, MatterSim, OriginPro

Education

2027.06 School of Physics and Optoelectronic Engineering, **Guangdong University of Technology**
2024.09 M.S. Candidate in Materials Physics and Chemistry
2024.06 School of Chemical Engineering and Light Industry, **Guangdong University of Technology**
2020.09 B.S. in Applied Chemistry **(Exemption from graduate entrance examination)**

Honors & Awards

- Graduate Elite Talent Program, Guangdong University of Technology
- First-Class Graduate Scholarship (2024, 2024–2025), Guangdong University of Technology
- Third Prize, South China Undergraduate Physics Experiment Competition (2022)
- Second Prize, Guangdong Division of the National Mathematical Contest in Modeling (2022)
- Outstanding Student Scholarship (2020–2023), Guangdong University of Technology

Research Experience

present – 2026.01 **CSP of Hydrogen-Based Superconductors via Multi-Objective Optimization** | GDUT
- Developed a multi-objective optimization framework integrating thermodynamic stability and superconducting properties into USPEX
- Establishing a closed-loop workflow of search–screen–validate–update
- Developed a web-based visualization and post-processing platform for USPEX

present – 2025.01 **CSP Driven by Universal Machine Learning Potentials** | GDUT
- Integrated universal ML potentials into USPEX for faster CSP
- Fine-tuned MatterSim to improve prediction accuracy under high pressure

2026.01 – 2025.01 **High-Throughput Screening of Conventional Superconductors** | GDUT
- Combined structure generators with MatterSim for high-throughput screening of hydrogen-based superconductors
- Accelerated substitution screening of layered boride superconductors using MatterSim

2026.01 – 2024.09 **Interpretable Prediction Model for T_c of Hydrogen-Based Superconductors** | GDUT
- Collected, preprocessed datasets and performed feature engineering
- Constructed interpretable models using SISSO
- Revealed relationships between pressure, electronic structure, and superconductivity

2024 – 2022 **Defect Engineering for Hydrogen Evolution Reaction in 2D Materials** | GDUT
- Systematically investigated the effects of defects on electronic structure and HER activity of HfX_2 (X = S, Se, Te)

Publications

- **Chen J**, Peng J, Liang Y, et al. Interpretable descriptors enable prediction of hydrogen-based superconductors at moderate pressures[J/OL]. *Materials Today Physics*, 2026, 63: 102073.(IF=9.7)
- Liang Y, **Chen J**, Huang Y, et al. High-Throughput Screening of Bulk Boride Superconductors with Honeycomb-Ruby Frameworks[J/OL]. *Inorganic Chemistry*, 2026, 65(10): 5731–5739.(IF=4.7)
- **Chen J**, Zhang R, Luo J, et al. Activating HfX_2 (X = S, Se and Te) for the hydrogen evolution reaction by introducing defects: a first-principles study[J/OL]. *Physical Chemistry Chemical Physics*, 2023, 25(38): 26043–26048.(IF=3.3)