Yiming Zhang

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PROFILE

Computational materials scientist and scientific software developer with experience in first-principles materials modelling, high-throughput workflow automation, HPC, and research software development. Experienced with DFT/DFPT, electron–phonon calculations, superconductivity, mechanical properties, and automated simulation workflows using Quantum ESPRESSO, EPW, and AiiDA. Strong Python development background with experience building workflow infrastructure, parsers, scientific databases, and LLM-assisted computational tools.

TECHNICAL SKILLS

Electronic structure: DFT, DFPT, phonons, electron–phonon coupling, Wannier interpolation, Eliashberg theory, elastic properties, stacking-fault energies
Scientific software: Quantum ESPRESSO, EPW, Wannier90, AiiDA, ASE, pymatgen
Programming: Python, Fortran, C++
Workflow & data: High-throughput computing, workflow automation, provenance tracking, scientific databases, REST/API-based scientific applications
HPC: Slurm, MPI, Linux, HPC workflows
AI & scientific applications: LLM integration, AI-assisted workflow execution, automated result analysis, scientific frontend/backend integration

EXPERIENCE

PhD Researcher – Computational Materials Science **2023 – Present**
UCLouvain, Belgium

- Developed automated first-principles workflows for high-throughput screening of superconducting and mechanically ductile materials.
- Performed DFT, DFPT, phonon, electron–phonon, and Eliashberg calculations using Quantum ESPRESSO and EPW.
- Built and maintained AiiDA workflows for automated structure relaxation, electronic structure, Wannierisation, phonons, superconductivity, and mechanical-property calculations.
- Developed Python tools for automated data analysis, convergence studies, provenance tracking, and extraction of physical properties from large computational datasets.
- Designed high-throughput computational protocols and executed large-scale simulations on European HPC systems.
- Investigated relationships between superconductivity and mechanical properties including elastic moduli, ductility descriptors, and generalized stacking-fault energies.

SELECTED SOFTWARE & RESEARCH PROJECTS

AiiDA–EPW Workflow Development *Python, AiiDA, EPW*

- Contributed to scientific workflow and parser development for automated electron–phonon and Eliashberg calculations.
- Improved parser robustness, explicit workflow interfaces, restart behaviour, and structured provenance of superconductivity data.
- Developed automated handling and analysis of EPW outputs for high-throughput superconductivity calculations.

High-Throughput Ductile Superconductor Screening *DFT, DFPT, AiiDA, Quantum ESPRESSO*

- Built automated workflows for screening superconductors using elastic properties, Pugh and Pettifor criteria, and stacking-fault energetics.
- Automated convergence studies and validation of mechanical and superconducting properties across hundreds of materials.
- Developed datasets and visualization infrastructure for publication and web-based dissemination of calculated materials properties.

LLM-Assisted Computational Materials Platform *Python, AiiDA, LLMs, Web Applications*

- Developed an experimental software platform connecting a frontend application, large language models, and AiiDA computational workflows.

- Designed tools for natural-language-driven job submission, workflow control, and automated interpretation of simulation results.
- Integrated computational workflow execution with scientific software and data services.

PUBLICATIONS

- **Y. Zhang**, et al., "In Search of Novel Ductile Superconductors," manuscript / preprint, 2026.

*Equal contribution. Full publication list: Google Scholar.

EDUCATION

PhD in Computational Materials Science **2023 – 2027**
UCLouvain, Belgium

- Research focus: first-principles superconductivity, computational materials science, high-throughput simulation, and scientific workflow automation.

M.Sc. in Optical Engineering **2020 – 2023**
Fudan University, Shanghai, China

B.Sc. in Optoelectronic Information Science and Engineering **2016 – 2020**
Fudan University, Shanghai, China

AWARDS

- FRIA Fellowship, F.R.S.-FNRS, Belgium, 2023
- Outstanding Graduate Student of Shanghai, 2023