XIAOJUN ZHANG, PhD

Computational Science | *AI & Modeling for Materials and Imaging*
Boston, MA | +1 (617) 378-5825 | xzhang2365@gmail.com
Linkedin: www.linkedin.com/in/xiaojun-zhang-9b8495321

PROFILE

Cross-disciplinary scientist with a strong foundation in mechanical and materials engineering, specializing in AI-assisted computational modeling and imaging analysis. My experience spans from designing and fabricating micro/nano-structured materials for flexible electronics (MS) to developing AI-driven 3D reconstruction methods for graphene from low-dose TEM imaging (PhD). This combined background enables me to bridge experimental fabrication and computational modeling, applying AI, simulation, and data analysis to solve complex problems in materials and imaging science.

EDUCATION

Ph.D., Mechanical Engineering (Computational Materials Science) Sep 2019 – Sep 2025
City University of Hong Kong Hong Kong SAR

M.S., Mechanical Engineering (Micro/Nano Fabrication of Functional Materials) 2016 - 2019
Xi'an Jiaotong University Xi'an, China

B.S., Mechanical Engineering 2021 - 2016
Northwest A&F University Xi'an, China

- GPA: 3.65
- Award: President Scholarship, National Scholarship, Merit Student & First-Class Scholarship

SKILLS

- **Computational & AI Tools:** Python, MATLAB, R, TensorFlow, PyTorch, scikit-learn
- **Modeling & Simulation:** Molecular Dynamics (LAMMPS), DFT (VASP), Simulated Annealing, Optimization
- **Imaging & Analysis:** TEM Data Processing (Tempas, StatSTEM), Image Reconstruction, Statistical Modeling, Signal Processing
- **Experimental & Design:** Micro/Nano Fabrication, Transfer Printing, Sensor Characterization
- **Software & Design Tools:** Pymol, Vesta, AutoCAD, SolidWorks, ProE

RESEARCH EXPERIENCE

PhD Researcher – Computational Materials & Imaging (City University of Hong Kong)
2019-2025

- Developed and implemented **machine learning methods** and **imaging processing tools** to denoise and preprocess high-time-resolution TEM datasets, enabling the detection and visualization of dynamic behaviors (e.g., rippling and curvature changes) in graphene induced by electron excitation.
- Applied **statistical parameter estimation techniques**, including **Maximum Likelihood (ML)** and **Bayesian estimators**, to estimate the initial 3D atomic positions from preprocessed low-dose TEM images.
- Developed **computational pipelines** for processing noisy, high-dimensional imaging datasets, leveraging **optimization tools** (e.g., Simulated Annealing) and **Molecular Dynamics (MD)** to reconstruct 3D atomic structures with sub-angstrom accuracy.
- Applied **Kullback-Leibler (KL) divergence** and other statistical measures to compare pixel intensity distributions, quantifying differences in noisy imaging datasets and improving the robustness of image analysis under varying conditions.

Research Assistant – Micro/Nano Fabrication (Xi'an Jiaotong University)

2016-2019

- Designed and fabricated flexible electronic devices using micro/nano patterning and transfer printing.
- Characterized piezoelectric sensors, achieving enhanced signal stability and mechanical flexibility.
- Collaborated with interdisciplinary teams to optimize material performance for electronic applications.

PUBLICATION

- **X. Zhang,** et al. "Atomic Resolution 3D Dynamics Retrieval of Graphene from High-speed Low-dose Data"**,** Manuscript in prep.

THESIS TOPIC

- **Ph.D**.: Three-dimensional Atomic Structure Reconstruction and Dynamic Analysis of Graphene using High-speed Low-dose TEM Imaging
- **M.S**.: Nanoscale Transfer Printing of Functional Materials for Flexible Electronic Devices
- **B.S**.: Nanostructured Flexible Piezoelectric Sensor Manufacturing and Performance Testing