XIAOJUN ZHANG, PhD

Computational Scientist | Image Processing | Machine Learning Specialist
Boston, MA | +1 (617) 378-5825 | xzhang2365@gmail.com
LinkedIn | GitHub | Website

PROFESSIONAL SUMMARY

Computational scientist with 6+ years of research experience in machine learning, computer vision, algorithm development, and statistical modeling for complex, high-dimensional datasets. Expert in developing computational pipelines for image analysis, 3D reconstruction, signal processing, and large-scale data processing. Strong background spanning computational science, materials science, mechanical engineering and experimental research with proven ability to bridge theory and practice.

TECHNICAL SKILLS

Programming & Analysis
Python, MATLAB, R, Git, Linux

Machine Learning & AI
PyTorch, TensorFlow, Statistical Learning, Computer Vision

Statistical Methods
Bayesian Inference, Maximum Likelihood Estimation, Monte Carlo Methods, KL Divergence

Computational Methods
Optimization Algorithms, Simulated Annealing, Molecular Dynamics (LAMMPS), DFT (VASP)

Imaging & Simulation
TEM Imaging (Tempas), STEM Imaging (StatSTEM)

Design & Modeling
AutoCAD, SolidWorks, PyMOL, VESTA, CouldCompare

PROFESSIONAL EXPERIENCE

PhD Research Scientist

City University of Hong Kong | Hong Kong *Sep 2019 – Sep 2025*

Research Focus: Computational Pipeline for Atomic Structure Reconstruction & Dynamic Analysis of Graphene

- **Developed novel computational framework** combining image processing, machine learning, model-based estimation theory, surface fitting, optimization methods and Molecular Dynamics for 3D atomic structure reconstruction of graphene from 2D low-dose TEM images, achieving sub-angstrom accuracy (0.45Å in z-direction), significantly outperforming existing methods
- **Captured and analyzed 3D atomic dynamics** of graphene ripples with high temporal resolution by combining single-shot reconstruction with sequential imaging, revealing electron beam-induced structural evolution and defect formation mechanisms
- **Investigated structure-property relationships** using Density Functional Theory (DFT) calculations to correlate 3D atomic geometries with electronic properties, providing insights into how structural distortions influence material behavior
- **Automated large-scale data processing pipeline** handling 50,000+ images with batch processing, quality control, and parallel computing optimization

Research Assistant (Master's Program)

Xi'an Jiaotong University | Xi'an *Sep 2016 – Sep 2019*

Research Focus: Micro-nano Manufacturing & Flexible Electronics

- **Designed and fabricated micro-nanostructured flexible sensors** achieving 2-3× performance improvement over conventional designs through innovative liquid-bridge transfer printing method

- **Developed novel fabrication process** enabling high-aspect-ratio structures (4:1, 200μm height) for supercapacitor electrodes using organic solvent displacement filling, significantly improving device capacitance
- **Engineered force-heat integrated sensors** for 3D curved surfaces combining piezoelectric and thermal sensing capabilities, demonstrating expertise in multi-functional device integration
- **Characterized device performance** through comprehensive testing protocols (CV curves, GCD curves, EIS analysis) and statistical data analysis using Origin Pro, VersaStudio, and custom MATLAB scripts

Teaching Assistant

City University of Hong Kong | Hong Kong

- MNE3007: CAD/CAM *2022/2023 Sem A*
- MNE6125 & MNE8108: Engineering Methods *2022/2023 Sem A*

EDUCATION

Ph.D., Computational Materials Science Sep 2019 – Sep 2025

City University of Hong Kong

- **Specialization**: Machine Learning, TEM Imaging, Simulation, Statistical Modeling
- **Thesis**: "3D Atomic Structure Reconstruction and Dynamic Analysis of Graphene using High-speed Low-dose TEM Imaging"

M.S., Mechanical Engineering Sep 2016 – Jul 2019

Xi'an Jiaotong University

- **Specialization**: Micro-nano Manufacturing, Experimental Design, Flexible Electronics
- **Thesis**: "Nanoscale Transfer Printing of Functional Materials for Flexible Electronic Devices "

B.S., Mechanical Engineering Sep 2012 – Jul 2016

Northwest A&F University

- **Major**: Mechanism Design, Manufacturing and Automatization
- **GPA**: 3.65/4.0 (89.2/100) | **Class Rank:** 3/195 (Top 2%)
- **Thesis**: "Nanostructured Flexible Piezoelectric Sensor Manufacturing and Performance Testing", recognized as an excellent paper at the university level

AWARD & PUBLICATION

- **X. Zhang,** et al. "Atomic Resolution 3D Dynamics Retrieval of Graphene from High-speed Low-dose Data" *(Manuscript in preparation)*
- **Award**: President Scholarship (2014), National Scholarship (2013), University-level Merit Student (2013~2016), University-level Professional First-class Scholarships (2013~2016)

EXTRACURRICULAR ACTIVITES

- Training on Micro-nano Manufacturing Experiments, *Xi'an Jiaotong University* 2016
- Debate Team Leader, *Northwest A&F University* 2014 - 2015
- Standard Chartered Hong Kong Marathon 2024 (Full Marathon) with a time of 4:16:34 2024
- Standard Chartered Hong Kong Marathon 2023 (Half Marathon) with a time of 2:09:14. 2023

ADDITIONAL INFORMATION

- **Work Authorization**: Active Employment Authorization Document (EAD) for USA
- **Language**: English (Fluent), Mandarin (Native)
- **Interests**: Reading, Jogging, Tennis, Piano, Hiking