XIAOJUN ZHANG, PhD

Computational Scientist | TEM Imaging | Machine Learning

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PROFESSIONAL SUMMARY

Computational Scientist with 6+ years of research experience in machine learning, algorithm development, and statistical modeling for complex, high-dimensional datasets. Skilled in developing computational pipelines to reconstruct 3D atomic structures from low-dose TEM images and characterize material properties. Complementing my computational expertise, I have 3+ years of hands-on experience in macro-nano fabrication and testing of flexible electronic devices. My interdisciplinary research spans mechanical engineering, computational science, and materials science, bridging experimental techniques and computational methodologies to address complex scientific challenges.

TECHNICAL SKILLS

Programming & Analysis

Python, MATLAB, R, NumPy, SciPy, Pandas, scikit-learn, Git, Linux/Unix

Machine Learning & AI

PyTorch, TensorFlow, Deep Learning, Statistical Learning, Feature Extraction, Pattern Recognition

Statistical Methods

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

Computational Methods

Simulated Annealing, Global Optimization, Molecular Dynamics (LAMMPS), DFT (VASP)

Data Processing & Visualization

Image Processing, Signal Processing, Denoising Algorithms, Matplotlib, Data Visualization

Design & CAD Tools

AutoCAD, SolidWorks, PyMOL, VESTA, HPC Computing Platforms

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

- **Developed novel computational framework** for 3D atomic structure reconstruction from 2D low-dose TEM images, achieving sub-angstrom accuracy (0.45Å in z-direction) using advanced Simulated Annealing

optimization—significantly outperforming existing methods

- **Pioneered integrated ML pipeline** combining statistical inference (Maximum Likelihood, Bayesian methods), physics-based simulations (Molecular Dynamics), and deep learning for structural analysis of low-dimensional materials with extremely low signal-to-noise ratios

- **Developed statistical framework using KL divergence** to quantitatively assess image quality under varying electron doses, establishing critical dose thresholds for meaningful structural analysis—providing guidelines for optimal low-dose imaging protocols

- **Applied advanced denoising techniques** (dictionary learning, sparse coding) to enhance signal-to-noise ratio in ultra-low-dose imaging, enabling detection of structural features previously obscured by noise—methodology directly applicable to noisy data domains

- **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, reducing analysis time from days to hours while maintaining accuracy

Research Assistant (Master's Program)

Xi'an Jiaotong University | Xi'an, China   *Sep 2016 – Jun 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

- **Built custom testing platforms** including variable-load signal acquisition systems for precise characterization of piezoelectric sensors and electrochemical workstations for supercapacitor performance evaluation

- **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

EDUCATION

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

City University of Hong Kong

Specialization: Machine Learning, Computational Science, Algorithm Development, 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: "Nanostructured Flexible Piezoelectric Sensor Manufacturing and Performance Testing"

Relevant Coursework: Finite Element Analysis, CAD/CAM/CAE, Robotics, Computational Methods, Micro-Nano Testing Technology, Nanomaterials, Micro-Nano Manufacturing Technology

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%)

Honors & Awards: President Scholarship, National Scholarship, Professional First-class Scholarships

Relevant Coursework: Mechanical Engineering, Engineering Graphics, Computer Programming Basics (C/C++), Computer Graphics

PUBLICATIONS

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

ADDITIONAL INFORMATION

Work Authorization: Active Employment Authorization Document (EAD) for USA
Languages: English (Fluent), Mandarin (Native)
Location: Boston, MA – Actively seeking opportunities in computational science, data science, machine learning, materials, and related fields
Interests: Reading, Running, Tennis, Hiking