XIAOJUN ZHANG, PhD

AI/ML Engineer | Computer Vision | Computational Modeling

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PROFESSIONAL SUMMARY

Computational scientist with 5+ years of experience developing AI-driven solutions for imaging analysis and materials characterization. Expert in building end-to-end machine learning pipelines for noisy, high-dimensional data. Proven track record of combining deep learning, optimization algorithms, and physics-based modeling to solve complex engineering problems. Seeking opportunities in computer vision, AI research, or computational modeling.

Core Competencies: Computer Vision • Deep Learning • Image Processing • Statistical Modeling • Algorithm Development • Python/PyTorch • Scientific Computing

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TECHNICAL SKILLS

Programming & AI/ML: Python, MATLAB, R, PyTorch, TensorFlow, scikit-learn, NumPy, SciPy
Computer Vision & Image Processing: TEM Data Processing, Image Reconstruction, Denoising Algorithms, Feature Extraction, Statistical Image Analysis
Modeling & Simulation: Molecular Dynamics (LAMMPS), DFT (VASP), Simulated Annealing, Optimization Algorithms, Monte Carlo Methods
Data Analysis: Statistical Inference, Bayesian Methods, Maximum Likelihood Estimation, KL Divergence, Signal Processing
Tools & Platforms: Git, Linux, AutoCAD, SolidWorks, Visualization (Matplotlib, Pymol, Vesta)
Domain Expertise: Materials Science, Nanofabrication, Sensor Design, Flexible Electronics

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PROFESSIONAL EXPERIENCE

PhD Research Scientist | City University of Hong Kong | Hong Kong

Computational Materials Science & AI-Driven Imaging | Sep 2019 – Sep 2025

AI/ML & Computer Vision:

- **Built end-to-end ML pipeline** for 3D atomic structure reconstruction from noisy TEM images, achieving **0.45Å (sub-angstrom) accuracy** in z-direction positioning—significantly outperforming traditional methods
- **Applied denoising algorithm** using dictionary learning and sparse coding, improving signal-to-noise ratio and enabling detection of atomic-scale dynamics in real-time
- **Implemented statistical estimation framework** combining Maximum Likelihood and Bayesian inference to extract 3D atomic coordinates from 2D projection images with **50000+ image dataset**
- **Designed optimization pipeline** integrating Simulated Annealing with Molecular Dynamics validation, processing high-dimensional data to ensure physically valid atomic configurations

Data Analysis & Modeling:

- **Applied KL divergence and statistical metrics** to quantify image quality degradation under varying electron doses, establishing minimum dose thresholds for reliable structural analysis
- **Processed high-speed, low-dose TEM datasets** to visualize dynamic behaviors (rippling, curvature changes) in graphene under electron beam excitation with temporal resolution
- **Integrated physics-based constraints** into ML models using Molecular Dynamics simulations, ensuring predictions aligned with physical laws and reducing false positives
- **Automated data pipeline** for batch processing of TEM images, reducing analysis time from days to hours

Technical Tools: Python (PyTorch, scikit-learn, NumPy, SciPy), LAMMPS, VASP, MATLAB, Statistical Modeling, Image Processing

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Research Assistant | Xi'an Jiaotong University | Xi'an, China

Micro/Nano Fabrication & Sensor Development | Sep 2016 – Jun 2019

Device Development & Optimization:

- **Designed and fabricated flexible piezoelectric sensors** with micro-nanostructured arrays, achieving **2-3× capacitance improvement** over conventional flat-film designs through innovative transfer printing process
- **Developed liquid-bridge transfer printing method** enabling fabrication of high-aspect-ratio structures (4:1, 200μm height), reducing manufacturing difficulty and production costs
- **Engineered supercapacitor electrodes** with structured CNT arrays, increasing surface area and improving energy storage performance through optimized micro-nano patterning

Experimental & Characterization:

- **Built custom testing platform** with variable-load signal acquisition system for precise measurement of sensor output under different conditions
- **Characterized electrochemical performance** using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS)

Materials & Processes: Piezoelectric materials (PVDF-TrFE, BTO-doped PVDF), CNTs, Graphene oxide, Ag conductive ink, PEDOT, PVA-H3PO4 electrolytes

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EDUCATION

Ph.D., Mechanical Engineering | City University of Hong Kong | Sep 2019 – Sep 2025
Specialization: Computational Materials Science, AI/ML for Imaging
Thesis: 3D Atomic Structure Reconstruction and Dynamic Analysis of Graphene using High-speed Low-dose TEM

M.S., Mechanical Engineering | Xi'an Jiaotong University | Sep 2016 – Jun 2019
Specialization: Micro/Nano Fabrication, Flexible Electronics
Thesis: Nanoscale Transfer Printing of Functional Materials for Flexible Electronic Devices

B.S., Mechanical Engineering | Northwest A&F University | Sep 2012 – Jun 2016
GPA: 3.65/4.0 (Top 2% of class)
Honors: President Scholarship, National Scholarship, First-Class Scholarship (multiple years)

PUBLICATIONS & PRESENTATIONS

- **X. Zhang**, et al. "Atomic Resolution 3D Dynamics Retrieval of Graphene from High-speed Low-dose Data" *(Manuscript in preparation)*
- Attended: International Conference on Intelligent Robotics and Applications, Wuhan, China (2017)

ADDITIONAL INFORMATION

Work Authorization: Active EAD (Employment Authorization Document) for USA
Languages: English (Fluent) Mandarin (Native)
Location: Boston, MA

KEY PROJECTS PORTFOLIO

3D Atomic Structure Reconstruction from Low-Dose TEM Imaging (2019-2025)

- Developed AI-driven pipeline combining machine learning, statistical inference, and physics-based optimization
- Technologies: Python, PyTorch, Simulated Annealing, Molecular Dynamics, Statistical Modeling
- Impact: Enabled sub-angstrom 3D reconstruction from single noisy images where traditional methods failed

Flexible Piezoelectric Sensor Design (2016-2019)

- Created micro-nanostructured sensors with 2-3× performance improvement
- Technologies: Micro/nano fabrication, Transfer printing, Electrochemical characterization
- Impact: Reduced manufacturing costs while improving sensor performance and mechanical flexibility

Structured Electrode Supercapacitor Development (2017-2019)

- Engineered high-aspect-ratio CNT electrode arrays for energy storage
- Technologies: Nanofabrication, PEDOT filling, Electrochemical testing
- Impact: Demonstrated significant capacitance increase through innovative structural design