CHENHAOYUE WANG | wchy97@g.ucla.edu | (510) 7354909 | linkedin.com/in/chenhaoyue-wang
Open to Relocate | MSE Ph.D. in Computational and Experimental Design of Solid-State, Energy, and Electronic Materials

EDUCATION

University of California, Los Angeles (UCLA) Sep 2021 – Jun 2026 (expected)
Ph.D. Candidate, Materials Science & Engineering, **Nanomaterials 2025 Travel Award** (2025)
GPA: 3.88/4.00 | Focus*: Computational modeling and theoretical studies of 2D and energy materials (DFT, MD, COMSOL, ML); electronic, thermal, and mechanical reliability in solid-state systems.*

Soochow University Sep 2015 – Jul 2019
*B.Eng. in New Energy Materials and Devices (**Highest Honor**)*, **Outstanding Graduate** (2019)
GPA: 3.70/4.00 (Major: 3.80/4.00), Rank: 4/120 | Focus: Li-ion batteries and electrochemical testing

TECHNICAL SKILLS

Simulation & Modeling: DFT (Quantum ESPRESSO, SPARC, ABINIT), MD (LAMMPS) for diffusion, defect energy, and thermal stability, COMSOL Multiphysics for electro-thermal and mechanical modeling.
Programming & Data: Python (NumPy, SciPy, Matplotlib, ASE, Numba, Ray, Scikit-learn) for data analysis, MATLAB and workflow automation, visualization (VESTA, Ovito), large-scale HPC runs (MPI and SLURM).
Machine learning: Data pre-processing, feature extraction, regression modeling for property prediction.
Battery & Experimental: Li-ion electrode fabrication, battery design, battery assembly, CVD synthesis, electrochemical testing (EIS, CV, charge-discharge cycling), SEM, Raman, glovebox operation.

RESEARCH EXPERIENCE – Simulation Materials

Strain-Engineered Flat-Band Silicon Kagome Lattice (SiKL) *UCLA* | 2021 – present
• Performed simulations to investigate the strain-dependent electronic properties (DFT), phonon dispersion (DFPT), thermal stability (AIMD), and mechanical resilience (MD) of silicon Kagome lattices across both small and large scales.
• Applied phonon-eigenvector perturbations to resolve structural instabilities and discover two metastable buckled phases with tunable flat-band and mechanical characteristics under strain engineering.
• Built Python workflows (NumPy, ASE, SciPy) for RDF and potential-energy analysis of >10,000-atom MD datasets; constructed a strain-temperature phase diagram.
• Found a critical strain (≈ 2 %) that switches from disorder accumulation to strain-enhanced crystallinity and bonding.
• Modeled substrate-induced strain on Ag (111) showing 0.1 biaxial strain and stability up to 446 K; demonstrated tunable flat-band behavior and interfacial stability relevant to next-generation electronic and energy materials.

Nanotube Magnetism and ML-Based Property Prediction *UCLA* | 2023 – present
• Simulated doping/vacancy-induced magnetism and spin polarization in P_2C_3 nanotubes under strain; analyzed thermal stability with AIMD simulations. ***Preprint: arXiv:2501.11239***
• Compiling datasets of structural, mechanical and magnetic descriptors to train ML models predicting strain-defect-strain correlations in nanotube systems across various chirality and elements.

Flat-Band Transport & Polarization in Layered Materials *UCLA* | 2024 – present
• Developed tight-binding and time-dependent quantum transport models (Python, MATLAB) for 2D materials to study spin/charge conductivity under external fields. ***Preprint: arXiv:2510.03530***
• Modeled polarization and tacking fault energy for twisted hBN/graphene to evaluate stability of 2D heterostructures for energy storage and electronics. ***Preprint and Publication: arXiv:2510.01419; Mech. Mater. 2023***

RESEARCH EXPERIENCE – Battery Experiments

Template-Engineered Graphene Shells for Tunable Electrochemical Materials Soochow University
Project Leader | National Undergraduate Innovation Program (¥10 000); 1st Prize Commercial Competition
• Designed and synthesized multilayer graphene shells (10-200 nm) via hard-template CVD, systematically tuning particle size and growth time to study structure-property relationships in electrochemical materials.
• Characterized morphology, porosity, and graphitization using SEM, TG, Raman, BET, FTIR, establishing how synthesis parameters control shell thickness and Li^+ transport pathways, achieving +25 % capacity at 10 C and >90 % retention after 500 cycles with optimized growth condition and electrode composition.
• Modeled electro-thermal and ion-transport behavior in COMSOL to link structure and performance.

PRESENTATIONS

APS March Meeting (2023, 2025); MRS Spring Meeting (2024); USNCCM (2023, 2025)