JING LYU (吕静)

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RESEARCH INTERESTS

Computational and experimental materials science with a mechanism-first emphasis on defect chemistry, phase transitions, and structure–property relationships across functional materials. Specific interests include: **(i)** ferroelectric/piezoelectric oxides — domain engineering, defect-dipole hardening, and dopant-mediated MPB tuning in PZT-based and $BiFeO_3$-based systems; **(ii)** transition-metal luminescent materials — crystal-field engineering, and ferroelectric-coupled photophysics including electrically programmable circularly polarized luminescence (CPL); **(iii)** semiconductor surface science — atomic-scale growth, metallization, and field-induced phase transitions on Ge/Si substrates; and **(iv)** AI for Science — DFT-to-machine-learning interatomic potential (MLIP) pipelines for accelerated simulation of ferroelectric phase transitions and defect dynamics.

EDUCATION

National University of Singapore, Singapore — Aug 2018 – Oct 2022
Ph.D. in Chemistry (Semiconductor Surface Science) — GPA: 4.1/5.0

- Thesis: Atomic-scale growth, electronic structure, and field-induced phase transitions of metallic and molecular nanowires on Ge(001).
- Advisors: Prof. Guo Qin Xu (NUS, Chemistry) & Dr. Shuo-Wang Yang (A*STAR IHPC).
- Funding: NUS Research Scholarship (full Ph.D. stipend, 2018–2022).

Xi'an Jiaotong University, Xi'an, China — Sep 2015 – Jul 2018
M.Eng. in Materials Science & Engineering — GPA: 3.67/4.0

- Thesis: Modulation of Quenched Bismuth Ferrite Ceramics by Defects.
- Advisor: Prof. Jiagang Wu.

Sichuan University, Chengdu, China — Sep 2011 – Jun 2015
B.Sc. in Materials Physics — GPA: 3.75/4.0

RESEARCH EXPERIENCE

Research Fellow, NUS Chongqing Research Institute & National University of Singapore — Mar 2023 – Present

- **Doped PZT-based piezoelectric ceramics — defect chemistry and phase-structure engineering.** Established a dual-mechanism narrative for PMN–PZT combining (i) MPB→T-phase shift that suppresses polarization rotation and (ii) defect-complex hardening.
- **Piezochromic hybrid halides — order/disorder mechanism.** Defended a ferroelectric order–disorder phase-transition mechanism (pyridinium rotational freezing) for piezochromism. Built a Python AIMD-analysis toolkit (dipole vectors, ring-plane SVD, $MnBr_4$ bond-angle variance, H-bond tracking) and designed a pressure-stratified CHGNet fine-tuning workflow with layer-freezing strategy.
- **AI4S / MLIP fine-tuning pipeline.** Established a DFT-to-MLIP fine-tuning workflow on CHGNet for ferroelectric phase-transition simulation.
- **Electrode-material interface engineering.** Co-led design of ferroelectric-nanoparticle coatings ($BaTiO_3$) on MXene anodes and lattice-coherent surface layers on high-voltage $LiCoO_2$ cathodes, improving chemical stability and ion-transport kinetics.
- **Mentoring.** Co-supervised students on project design, computational methodology, and manuscript preparation.

Ph.D. Researcher, Department of Chemistry, National University of Singapore Aug 2018 – Oct 2022
*Joint with Institute of High Performance Computing (IHPC), A*STAR | Singapore*

- **Surface metallization of Ge(001).** Resolved the atomic-scale nucleation, diffusion, and self-assembly of Au-, Pt-, and Cu-induced nanowires on Ge(001) by combining UHV-STM imaging with first-principles (DFT) calculations; established physically grounded growth models relevant to nanoscale interconnect electromigration and thermal stability.
- **Field-induced phase transitions on semiconductor surfaces.** Demonstrated reversible STM-tip-driven structural phase transitions of surface nanowires; quantified metastable energy barriers by DFT and validated a field-driven switching mechanism with relevance to non-volatile memory.
- **Molecular nanowires on pre-patterned Ge(001).** Fabricated TCNQ-based molecular nanowires anchored to pre-patterned Ge(001) inorganic templates via PVD/MBE; combined STM and DFT to resolve adsorption geometry, charge transfer, and 1D electronic structure.
- **High-T surface dewetting and alloying.** Characterized dewetting and silicide/germanide alloying under high-temperature annealing, with implications for back-end-of-line (BEOL) thermal processing.

Graduate Researcher, Xi'an Jiaotong University, Xi'an, China Sep 2015 – Aug 2018
Advisor: Prof. Jiagang Wu

- **Defect engineering in $BiFeO_3$ lead-free ferroelectrics.** Controlled oxygen-vacancy concentration via Sm/Sc co-doping; reduced leakage current and resolved high-temperature dielectric breakdown.
- **Defect-dipole-induced poling.** Established that quenching-induced defect dipoles enable a strain-memory effect and enhance piezoelectric response in $BiFeO_3$-based ceramics.

TECHNICAL EXPERTISE

First-principles & atomistic computation: VASP (AIMD, CI-NEB, defect supercells with FNV charge correction, ΔSCF excited-state), Quantum ESPRESSO, CP2K, Gaussian, Materials Studio.

Machine-learning interatomic potentials: CHGNet fine-tuning with stratified train/val/test splitting, layer-freezing strategy; DFT-to-MLIP training-data pipelines.

Spectroscopy & characterization: EPR, XRD/Rietveld refinement, BSE, PFM, P–E / S–E hysteresis loops, dielectric spectroscopy, STM/STS (UHV).

Experimental fabrication: UHV-MBE/PVD for nanostructure growth on semiconductor surfaces; conventional and quenching-based ceramic sintering; battery-electrode preparation.

Programming & workflow: Python, Linux/HPC, VASP workflow automation, custom AIMD analysis toolkits, Bash.

Scientific graphics: Adobe Illustrator, Adobe Photoshop, Cinema 4D.

PUBLICATIONS

Over 30 SCI publications | 16 first-author / co-first / corresponding-author

First-Author / Co-First-Author / Corresponding-Author Publications

1. Guo, H.; Zhang, X.; **Lyu, J.** (co-first author); et al. Versatile construction of high-loading asymmetrically coordinated transition-metal single atoms for efficient ammonia electrosynthesis. *Nature Synthesis*, **2026**, 1-11.
2. Li, X.; … **Lyu, J.** (corresponding author); et al. Epitaxially grown lattice-coherent surface enabling superior mechanical integrity for high-voltage $LiCoO_2$ cathode. *Angewandte Chemie International Edition*, **2025**, e202504221.
3. Tian, M.; **Lyu, J.** (corresponding author); Su, R.; Zhang, X.; et al. Harnessing the power of nano-ferroelectrics: $BaTiO_3$/MXene ($Ti_3C_2T_x$) composites for enhanced lithium storage. *Advanced Energy Materials*, **2024**, 14, 2401988.

4. Li, X.; **Lyu, J.** (corresponding author); et al. Integrated optimization design with inherent element behaviors for bulk and surface stability toward 4.7 V $LiCoO_2$ cathode. *Nano Energy*, **2024**, 110496.
5. Zhang, X.; Wang, K.; Qiu, J.; Tian, M.; Guo, H.; Yang, S.; **Lyu, J.** (corresponding author); Xu, G. Low-cobalt single atoms loading on N-doped carbon for high Na-storage performance. *Nano Energy*, **2024**, 129, 110018.
6. Wang, X.; **Lyu, J.** (corresponding author); et al. Engineered composite interfacial electric field boosts piezocatalysis of perovskite ferroelectrics. *ACS Applied Materials & Interfaces*, **2024**, 16, 52624.
7. **Lyu, J.**; Wong, Z. M.; Sun, H.; et al. Self-assembled molecular nanowires on prepatterned Ge(001) surfaces. *Chemical Science*, **2022**, 13(19), 5674–5679.
8. **Lyu, J.**; Wong, Z. M.; Sun, H.; et al. Electric-field-induced phase transition of nanowires on Ge(001) surfaces. *The Journal of Physical Chemistry Letters*, **2022**, 13, 1063–1068.
9. **Lyu, J.**; Wong, Z. M.; Sun, H.; et al. Uncovering the self-organized nanowires on Au-modified Ge(001) surfaces. *The Journal of Physical Chemistry C*, **2021**, 125(50), 27876–27883.
10. **Lyu, J.**; et al. Deciphering the growth mechanism of self-assembled nanowires on Pt-deposited Ge(001) via STM and DFT calculations. *The Journal of Physical Chemistry C*, **2020**, 124, 18165–18172.
11. **Lv, J.**; Gao, W.; Li, J.; et al. Large strain and strain-memory effect in bismuth-ferrite lead-free ceramics. *Journal of Materials Chemistry C*, **2017**, 5, 9528–9533.
12. **Lv, J.**; Zhao, H.; Wu, M.; et al. Modulating the electric and magnetic properties of $BiFeO_3$ ceramics. *Materials & Design*, **2017**, 125, 213–221.
13. **Lv, J.**; Lou, X.; Wu, J. Defect-dipole-induced poling characteristics and ferroelectricity of quenched bismuth-ferrite-based ceramics. *Journal of Materials Chemistry C*, **2016**, 4(25), 6140–6151.
14. **Lv, J.**; Wu, J.; Wu, W. Enhanced electrical properties of quenched $(1–x)Bi_{1–y}Sm_yFeO_3–xBiScO_3$ lead-free ceramics. *The Journal of Physical Chemistry C*, **2015**, 119(36), 21105–21115.

Selected Co-Author Publications

15. Wang, M.; Zhang, Z. B.; **Lyu, J.**; Qiu, J.; Gu, C.; Zhao, H.; Wang, T.; Ren, Y. W.; Yang, S. W.; Xu, G. Q.; Liu, X. G. Overcoming thermal quenching in X-ray scintillators through multi-excited-state switching. *Angewandte Chemie International Edition*, **2024**, 63, e20240194.

A complete list of co-author publications spanning surface electrochemistry, lead-free piezoelectrics, and oxide thin films is available on Google Scholar.

AWARDS & HONORS

- **NUS Research Scholarship** — National University of Singapore (2018–2022)
- **National Scholarship for Graduate Students** — Ministry of Education, China (2017)
- **Outstanding Graduate Student Model** — Xi'an Jiaotong University (2017)
- **Outstanding Graduate Student** — Xi'an Jiaotong University (2016)
- **Outstanding University Graduate of Sichuan Province** — Province of Sichuan, China (2015)
- **National Encouragement Scholarship** — Ministry of Education, China (2013, 2014)
- **National Scholarship** — Ministry of Education, China (2012)
- **First-Class Comprehensive Scholarship** — Sichuan University (2012)

REFERENCES

Available upon request.