Yongxin Lyu

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Profile

- Computational materials scientist specialised in data-driven materials discovery, multiscale materials modeling for optoelectronic applications.
- 10 publications in peer review journals including Nature Materials, Advanced Materials, Applied Physics Letters; 650+ citations, h-index: 9.
- Completed research training in experiment research groups; skilled in bridging the gap between computational modeling and experimental realisation.
- Developed a data-driven workflow that shortlisted 55 new materials from 4 millions candidates; contributed to course content design for a data science course in chemical engineering

Education

University of New South Wales (UNSW), PhD in Materials Science & Engineering — Jun 2021 – Aug 2025

- Thesis: AI-assisted inverse design of two-dimensional hybrid perovskites

The Hong Kong Polytechnic University, MPhil in Physics — Sep 2017 – May 2020

- Thesis: Lanthanide near-infrared luminescence in layered semiconductor nanosheet hosts

The Hong Kong Polytechnic University, BSc in Physics — Sep 2013 – May 2017

- First class Honors; Dean's Honours List 2016

Research Experience

Professor Tom Wu's group | UNSW — Jun 2021 – Aug 2025

Data-driven discovery of organic-inorganic hybrid materials

- Developed a AI-assisted materials discovery workflow combining high-throughput DFT, ML models, and synthesis feasibility analysis to screen 4 million candidates and propose 55 new 2D perovskites with target electronic properties.
- Accelerated 2D perovskites discovery by enabling inverse-design of candidates from a target electronic properties, reducing experimental trial and errors.
- Collaborated with experimentalists to encode feasibility criteria that guided shortlisting toward experimentally realizable compounds.

Professor Jianhua Hao's group | The Hong Kong Polytechnic University — Sep 2017 – Jan 2021

Multiscale modeling of 2D materials

- Investigated synthesis processes and near-infrared lanthanide luminescence in doped 2D materials using first-principles modeling.
- Studied the mechanisms of large-scale black phosphorus growth through molecular dynamics simulations.
- Collaborated across 5 experimental projects on various 2D materials families and applications.

Publications

Yongxin Lyu, Yifan Zhou, et. al. (2025). Fingerprinting organic molecules for the inverse design of two-dimensional hybrid perovskites with target energetics, In revision, Science Advances, 10.48550/arXiv.2509.25728

Yongxin Lyu, Zehan Wu, et. al. (2019). Observation and theoretical analysis of near-infrared luminescence from CVD grown lanthanide Er doped monolayer MoS_2 triangles, Applied Physics Letters, 10.1063/1.5120173

Zehan Wu, **Yongxin Lyu**, et. al. (2021). Large-scale growth of few-layer two-dimensional black phosphorus, Nature Materials, 10.1038/s41563-021-01001-7

Ran Ding, **Yongxin Lyu**, et. al. (2021). Effective piezo-phototronic enhancement of flexible photodetectors based

on 2D hybrid perovskite ferroelectric single-crystalline thin-films, Advanced Materials, 10.1002/adma.202101263

Ran Ding, **Yongxin Lyu**, et. al. (2022). Revealing photovoltaic behavior in 2D hybrid perovskite ferroelectric single-crystalline microwire arrays for self-powered photodetectors, Materials Today Physics, 10.1016/j.mtphys.2022.100867

Menglin Song, **Yongxin Lyu**, et. al. (2021). One-step, DNA-programmed, and flash synthesis of anisotropic noble metal nanostructures on MXene, ACS Applied Materials & Interfaces, 10.1021/acsami.1c16377

Gongxun Bai, **Yongxin Lyu**, et. al. (2020). Lanthanide near-infrared emission and energy transfer in layered WS_2/MoS_2 heterostructure, Science China Materials, 10.1007/s40843-019-1232-2

Feng Guo, **Yongxin Lyu**, et. al. (2020). Piezoelectric biaxial strain effects on the optical and photoluminescence spectra of 2D III–VI compound α-In_2Se_3 nanosheets, Applied Physics Letters, 10.1063/5.0001795

Yuan Liu, Gongxun Bai, **Yongxin Lyu**, et. al. (2020). Ultrabroadband tuning and fine structure of emission spectra in lanthanide Er-doped ZnSe nanosheets for display and temperature sensing, ACS Nano, 10.1021/acsnano.0c07547

Zhibin Yang, Zehan Wu, **Yongxin Lyu**, et. al. (2019). Centimeter-scale growth of two-dimensional layered high-mobility bismuth films by pulsed laser deposition, InfoMat, 10.1002/inf2.12001

Skills

- **Multi-scale materials modeling**: Expertise in first-principles simulation (VASP, Quantum ESPRESSO, Gaussian) and molecular dynamics simulation (LAMMPS).
- **High-throughput computing & workflow**: Extensive experience with Bash scripting and Linux-based workflows on national HPC systems (Gadi, Setonix).
- **Machine learning & AI**: Application of supervised and unsupervised learning methods using scikit-learn and PyTorch for data-driven materials discovery.
- **Scientific visualisation**: Creation of high-quality figures and animations using matplotlib, seaborn, plotly, Inkscape, ChemDraw, Blender.

Teaching Experience

Teaching Assistant | UNSW Chemical Engineering — Jun 2025 - present

- Course content developer: *Data-driven decision making for Chemical engineering and food science*.
- Curated real-world datasets from industry and research papers to strenghen the course's applied focus.
- Assisted students with machine learning and statistical modeling during tutorials.

Mentor and Tutor | Personalised English Language Enhancement (PELE), UNSW — Jan 2021 - present

- Delivered tutorials to 30+ undergrad, postgrad, and HDR students.
- Mentored 30+ HDR students in developing their personal project to improve English communication skills.
- Teacher satisfaction rate of 5.83/6 (97%); 88% response rate; Higher than the University average 5.44 (91%).

Funding and Awards

Research Training Program (RTP) PhD Scholarship: $131,100 across 3.5 years — 2021 - 2024

3rd Place, APAC HPC-AI Competition, Australia — 2022

STEMM Champions Program, UNSW — 2023

People's choice award, Materials Science & Engineering poster competition, UNSW — 2025

Volunteer Experience

Peer mentoring coordinator, School of Materials Science & Engineering, UNSW — 2023

Scientific blog writer, personal website — 2024 - present