Yongxin Lyu

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About Me

I am a materials scientist specializing in AI-assisted inverse design of 2D hybrid perovskites. My work combines machine learning, DFT simulations, and data-driven approaches to accelerate the discovery of novel materials for energy applications. I am passionate about computational modeling, automation workflows, and scientific outreach.

Education

University of New South Wales (UNSW) *Sydney, Australia*

Ph.D. in Materials Science and Engineering *June 2021 - July 2025*

- Thesis: AI-assisted inverse design of two-dimensional hybrid perovskites
- Supervisor: Prof. Tom Wu

The Hong Kong Polytechnic University *Hong Kong*

M.Phil. in Applied Physics *Sep 2017 - May 2020*

- Thesis: Lanthanide near-infrared luminescence in layered semiconductor nanosheet hosts
- Supervisor: Prof. Jianhua Hao

B.Sc. in Applied Physics (1st Class Honors) *Sep 2013 - May 2017*

Research Experience

AI-driven materials discovery *2021 - present*

University of New South Wales (UNSW), Prof. Tom Wu's Group

- Developed an AI-assisted materials discovery pipeline integrating first-principles simulations, machine learning, and synthesis feasibility analysis for the design of 2D hybrid perovskites.
- Inverse-designed novel 2D perovskite candidates targeting specific electronic properties and practical synthesis constraints.

Modeling and Synthesis of 2D Materials *2017 - 2021*

The Hong Kong Polytechnic University, Prof. Jianhua Hao's Group

- 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 via molecular dynamics simulations.

Publications

Fingerprinting Organic Molecules for the Inverse Design of Two-Dimensional Hybrid Perovskites with Target Energetics
Yongxin Lyu, Yifan Zhou, Yu Zhang, Yang Yang, Bosen Zou, Qiang Weng, Tong Xie, Claudio Cazorla, Jianhua Hao, Jun Yin, Tom Wu
Manuscript submitted. 2025

Effective piezo-phototronic enhancement of flexible photodetectors based on 2D hybrid perovskite ferroelectric single-crystalline thin-films
Ran Ding, Yongxin Lyu, Zehan Wu, Feng Guo, Weng Fu Io, Sin-Yi Pang, Yuqian Zhao, Jianfeng Mao, Man-Chung Wong, Jianhua Hao
Advanced Materials p. 2101263. 2021

Large-scale growth of few-layer two-dimensional black phosphorus
Zehan Wu, Yongxin Lyu, Yi Zhang, Ran Ding, Beining Zheng, Zhibin Yang, Shu Ping Lau, Xianhui Chen, Jianhua Hao
Nature Materials pp. 1203–1209. 2021

Observation and theoretical analysis of near-infrared luminescence from CVD grown lanthanide Er doped monolayer MoS_2 triangles
Yongxin Lyu, Zehan Wu, Weng Fu Io, Jianhua Hao
Applied Physics Letter p. 153105. 2019

Teaching Experience

Teaching Assistant

UNSW - Data-driven Decision Making for Chemical Engineering *2025 Term 2*

- Developed Jupyter Notebook tutorials for data analysis using Python libraries(e.g., pandas, scikit-learn).
- Assisted students with machine learning and statistical modeling.

Tutor

UNSW - Personalised English Language Enhancement (PELE) *2025 Term 2*

- Guided students in improving their English communication skills.
- Supported students through the design and implementation of personal projects tailored to their individual language and academic goals.

Technical Skills

Programming & Data Analysis	Python (pandas, NumPy, matplotlib, seaborn, Plotly, Scikit-learn), Bash/Shell scripting.
Data Visualization & Graphics	seaborn, Plotly, Inkscape, ChemDraw, Blender.
Scientific Computing & Workflow	Git, GitHub, LaTeX, HPC environments.

Awards and Honors

2025 **Chemical Engineering Teaching Microgrant**, UNSW
2023 **STEMM Champions Program**, UNSW
2022 **Third Place, APAC HPC-AI Competition**, Australia
2021-2024 **Research Training Program (RTP) Scholarship**, Australian Government
2016 **Dean's Honours List**, PolyU Hong Kong

Public Engagement

Pint of Science Australia
Presenter- Fantastic Perovskites and where to find them *May 2023*

Science in the Swamp
Outreach demonstrator *Aug 2023*

Volunteering Experience

Graduate Mentor, Personalised English Language Enhancement (PELE) Program
Faculty of Arts and Social Sciences, University of New South Wales *Jan 2022 - Dec 2024*

Peer Mentor Coordinator, Postgraduate Student Society (PGSOC)
School of Materials Science and Engineering, University of New South Wales *Jan 2024 - Dec 2024*