Zongmin Zhang

HKUST Computer Science Undergraduate | AI for Science Researcher

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Website Scholar ORCID GitHub LinkedIn X

EDUCATION

The Hong Kong University of Science and Technology (HKUST) 09/2023 – present

School of Engineering (SENG) – Bachelor of Engineering (BEng) in Computer Science; Minor in Chemistry

CGA: 3.987/4.300 | Dean's List in all completed regular semesters | Awarded HKSAR Government Scholarship twice.

Selected A+ Coursework

Course title	Grade
PHYS1007 Quantum Information for Everyone	A+
CHEM1020 General Chemistry I	A+
CHEM1030 General Chemistry II	A+
CHEM2111 Fundamentals of Organic Chemistry	A+
COMP2011 Programming with C++	A+
COMP2012 Object-Oriented Programming and Data Structures	A+
COMP3021 Java Programming	A+
COMP3711 Design and Analysis of Algorithms	A+
COMP4451 Game Programming	A+
MATH2011 Introduction to Multivariable Calculus	A+
MATH2111 Matrix Algebra and Applications	A+
MATH2411 Applied Statistics	A+
MATH2421 Probability	A+

PUBLICATIONS & PREPRINTS

[1] **Zongmin Zhang**, Yuyang Lou, Bowen Zhang, Junwu Chen, Ryo Kuroki, Xuan Vu Nguyen, Edvin Fako, Lixue Cheng, and Philippe Schwaller. "AdsMind: A Physics-Grounded Multi-Agent System for Self-Correcting Discovery of Adsorption Configurations on Heterogeneous Catalyst Surfaces." *Journal manuscript under review; arXiv preprint arXiv:2606.19152*, 2026. **Sole first author.** Led the implementation, benchmark design and cross-backend evaluation of AdsMind, a closed-loop, physics-grounded multi-agent system for autonomous adsorption-configuration discovery on heterogeneous catalyst surfaces.

[2] Zhilong Song, **Zongmin Zhang**, and Lixue Cheng. "Autonomous Heterogeneous Catalyst Discovery with a Self-Evolving Multi-Agent Digital Twin." *Journal manuscript under review; arXiv preprint arXiv:2606.05050*, 2026. **Second author.** Conducted Codex-based ablation experiments and contributed to the evaluation of CatDT, a self-evolving multi-agent digital-twin framework for autonomous heterogeneous catalyst discovery.

[3] Aritra Roy et al. (including **Zongmin Zhang**). "From Knowledge to Action: Outcomes of the 2025 Large Language Model (LLM) Hackathon for Applications in Materials Science and Chemistry."

arXiv preprint arXiv:2605.03205, 2026. Large-author community report on LLM-enabled scientific workflows from an international hackathon at the intersection of large language models, materials science, and chemistry.

ACADEMIC & RESEARCH EXPERIENCE

Undergraduate Research Assistant (UGRA), AI for Physical Sciences (AI4PhySci) Lab, HKUST 02/2026 – present

Supervisor: Prof. Sherry Lixue Cheng

- Conducting AI for Science research on chemistry-oriented machine learning, multi-agent systems (MAS), and autonomous scientific discovery, leading to preprints on AdsMind and CatDT.

HKUST Undergraduate Research Opportunities Program (UROP) 02/2026 – 05/2026

Supervisor: Prof. Sherry Lixue Cheng

UROP Project: Developments and Applications of Orbital-Based Learning as a General and Accurate Property Predictor

Project Student, Laboratory of Artificial Chemical Intelligence (LIAC), Institute of Chemical Science and Engineering (ISIC), EPFL 09/2025 – 01/2026

Supervisors: Prof. Philippe Schwaller & Dr. Edvin Fako

- Completed a semester research project on agentic simulation of atomic rearrangement and surface reactivity, which initiated the collaboration with EPFL LIAC on AdsMind.

HKUST Undergraduate Research Opportunities Program (UROP) 02/2025 – 05/2025

Supervisor: Prof. Xiaojuan Ma

UROP Project: Assess User Experience to Design Effective Visual Representation and Interaction in Virtual Reality

HKUST Undergraduate Research Opportunities Program (UROP) 06/2024 – 12/2024

Supervisor: Prof. Raymond Chi-Wing Wong

UROP Project: Knowledge Discovery Over Database

HONORS & SCHOLARSHIPS

HKUST SENG Dean's List (Spring 2026, expected) 09/2026

HKSAR Government Scholarship Fund – Scholarship for Outstanding Performance for the 2025/26 academic year (HK$80,000) 12/2025

Hong Kong, China–Asia-Pacific Economic Cooperation Scholarship for the 2025/26 academic year 12/2025

HKUST Study Abroad Funding Support (HK$10,000) 12/2025

- HKUST Study Abroad Grant
- HKSAR Government Scholarship Fund – Reaching Out Award (ROA)

HKUST SENG Dean's List (Spring 2025) 09/2025

HKUST SENG Dean's List (Fall 2024) 02/2025

HKSAR Government Scholarship Fund – Scholarship for Outstanding Performance for the 2024/25 academic year (HK$80,000) 12/2024

Hong Kong, China–Asia-Pacific Economic Cooperation Scholarship for the 2024/25 academic year 12/2024

HKUST SENG Dean's List (Spring 2024) 09/2024

HKUST SENG Dean's List (Fall 2023) 02/2024

OVERSEAS EXCHANGE & INTERNATIONAL EXPERIENCE

HKUST SENG Undergraduate Outbound Exchange Student, École Polytechnique Fédérale de Lausanne (EPFL), School of Computer and Communication Science, Lausanne, Vaud, Switzerland 09/2025 – 02/2026

Association of Pacific Rim Universities (APRU) Virtual Student Exchange (VSE), hosted online by Shanghai Jiao Tong University (SJTU), School of Materials Science and Engineering, Shanghai, China 02/2025 – 06/2025

Relevant coursework: MSE2602 Materials Chemistry.

INDUSTRY & INTERNSHIP EXPERIENCE

Xuzhou Sansen Well Mining Technology Co., Ltd., Shanghai R&D Center 06/2025 – 08/2025

Computer Vision Algorithm Intern, Shanghai, China

Independently built an end-to-end multi-view 3D reconstruction pipeline for industrial wire-rope inspection.

Qingdao Virtual Reality Institute (QVRI) Co., Ltd. 12/2024 – 01/2025

Unity VR Development Intern, Qingdao, Shandong, China

Lucent Qingdao R&D Center 08/2024

Front-End Development Assistant, Qingdao, Shandong, China

TEACHING, ACADEMIC SERVICE & UNIVERSITY OUTREACH

Reviewer, ICML 2026 AI for Science Workshop (OpenReview) 2026

Student Representative, HKUST SENG Mainland Undergraduate Recruitment Trip for JEE Main Round Interview Mingling Sessions, Guangzhou, Guangdong, China 06/2026 – 07/2026

HKUST CSE Programming Commons Undergraduate Teaching Assistant (UGTA) 02/2026 – 05/2026

HKUST COMP2011 Programming with C++ Undergraduate Teaching Assistant (UGTA) 02/2025 – 05/2025

HKUST CSE Programming Commons Undergraduate Teaching Assistant (UGTA) 09/2024 – 12/2024

EXTRACURRICULAR ACTIVITIES & LEADERSHIP

Founding Organizer, HKUST AI for Chemistry Club, HKUST Department of Chemistry (DAG registration in progress) 2026 – present

Initiated a student-led academic community for seminars, reading groups, workshops, and peer learning at the intersection of artificial intelligence and chemistry.

Finalist Award (Team Category), HKUST GenAI Hackathon Competition on a Putonghua Web Tool 03/2026

First Prize, The 5th National University Students' Data Analysis Popular Science Knowledge Competition (Theory Track) 2026

Outstanding Volunteer, National University Students' Data Analysis Popular Science Knowledge Competition 2026

ADDITIONAL INFORMATION

Technical Skills

- **Programming languages:** C/C++ (proficient), Java (proficient), Python (proficient), Scala, C#, JavaScript, Rust
- **Deep Learning (DL):** NumPy, PyTorch (Python & C++), TensorRT
- **AI Agent:** LangChain, LangGraph, ReAct, Retrieval-Augmented Generation (RAG), Model Context Pro-

tocol (MCP), agent tool and skill design for Codex and Claude Code

- **Chemoinformatics:** RDKit, Atomic Simulation Environment (ASE)
- **Operating Systems:** Linux command line, shell scripting, OS internals, and kernel-level programming
- **Computer Vision (CV):** YOLO, SAM, 3D Reconstruction
- **Digital Image Processing (DIP):** OpenCV (Python & C++)
- **3D visualization:** Visualization Toolkit (VTK)
- **Web front-end development:** Streamlit
- **Game development:** Godot, Unity
- **XR (AR/VR) development:** Meta XR Development Toolkit

Language Proficiency

Mandarin (native); English (professional working proficiency, Gaokao English: 142/150); Japanese (approx. JLPT N3 level); French (approx. CEFR A1 level); Cantonese (basic)

Research Training

Responsible Conduct of Research (UROP), CITI Program, The Hong Kong University of Science and Technology Valid until 06/2029