Hanlin Wu

Phone/WeChat: +8618801005017 **Email:** leon_bit@163.com

EDUCATION

Tsinghua University, Beijing, China

PhD Student, Institute for Artificial Intelligence Industry Research (AIR)

Beijing Institute of Technology, Beijing, China

Bachelor in Artificial Intelligence, School of Computer Science and Technology

GPA: 92.8/100 Rank: 1/71

English Proficiency: CET6: 578/710 IELTS: 7.5/9

Proficient: Generative Models (diffusion models, flow matching, Bayesian flow networks…)

AI for Scientific Discovery (protein, material, small molecules…)

Interested: Reinforcement Learning for Large Language Model

ACADEMIC PAPER

A Periodic Bayesian Flow for Material Generation [URL]

ICLR 2025 **Spotlight Paper, First Author**

- Achieved new state-of-the-art on all crystal generation benchmarks beating diffusion models with **~100x sampling efficiency**.
- Developed the first Bayesian flow in **non-Euclidean space** with a novel entropy conditioning mechanism tackling the unprecedented and pivotal non-additive accuracy theoretical challenge.

Rationalized All-Atom Protein Design with Unified Multi-Modal Bayesian Flow

NeurIPS 2025, **First Author**

- Identify and resolve the issues of **information shortcut** in all-atom protein generation with a novel rationalized information flow.
- Develop a new protein generation approach with Bayesian flow, by **transforming SO(3) generation** into an equivalent problem on **diffeomorphic hypersphere** with antipodal symmetry.
- Achieving superior performance compared to flow matching and diffusion baselines.

MOF-BFN: Metal-Organic Frameworks Structure Prediction via Bayesian Flow Networks

NeurIPS 2025, **Co-First Author**

- Build the first hierarchical structure prediction framework that jointly models periodicity, position, and orientation generating **thousands of atoms** using Bayesian flow networks.
- Incorporate fractional coordinates to capture periodicity and employ Bingham distributions to generate orientations in the unit quaternion space.

SCHOLARSHIP AND AWARDS

China National Scholarship 2022

Canada Mitacs Global Research Scholarship ($6375) 2023

First Prize in China Computer Federation Language Intelligence Contest (1/403, 20000CNY) 2023