

Junwen Liao

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Research Profile

Ph.D. candidate with training in mathematics, statistics, computational imaging, and AI for science. My current research focuses on multimodal integration of AlphaFold-style protein structure priors with cryo-EM observations, with broader interests in computational structural biology, inverse problems, generative models, and scientific machine learning.

Education

2024–Present	Ph.D. Candidate in Mathematics Advisor: Prof. Chenglong Bao.	Qiuzhen College, Tsinghua University
2020–2024	B.S. in Statistics Advisor: Prof. Zhiguo Wang. GPA: 3.89/4.00.	School of Mathematics, Sichuan University

Research Interests

AI for Science; Computational Imaging; Computational Structural Biology; Protein Structure Prediction; Generative Models; Inverse Problems.

Research Projects and Publications

2024.06–Present	Multimodal Integration of Cryo-EM and AlphaFold for Protein Structure Prediction Advisor: Prof. Chenglong Bao - Developed CoCoFold, a framework that adapts AlphaFold using limited cryo-EM particles to refine atomic models when reconstructed maps are weak, anisotropic, or incomplete. - Connected predicted atomic structures to experimental cryo-EM particles through differentiable density generation, projection, and particle-level supervision. - Designed target-specific refinement while preserving the AlphaFold structural prior, improving robustness in scarce-particle and missing-view regimes. - Continuing this direction through CoCoFold2, with emphasis on frozen protein-structure priors, target-specific latent correction, and broader experimental modalities. Publication: Junwen Liao*, Dihan Zheng*, Hui Zhang*, Linfeng Zhang, Mingxu Hu, and Chenglong Bao. "Fine-tuning AlphaFold with limited cryo-EM observations." <i>Communications Chemistry</i>, 2026. Paper / Code.
2023.08–2024.03	Deep Learning for Compressed-Sensing Computational Imaging Advisor: Prof. Chenglong Bao - Built a neural reconstruction framework for simulated integrated-circuit imaging by unrolling filtered back-projection and treating projection angles as learnable parameters. - Compared the proposed approach with traditional reconstruction algorithms and existing neural-network methods. - Achieved more accurate image reconstruction with a smaller parameter count, demonstrating a compressed-sensing imaging strategy. - Awarded Outstanding Undergraduate Thesis, Sichuan University.

2022.07–2023.04

Chemical Identification from Terahertz Absorption Spectra

Advisors: Prof. Zhiguo Wang and Prof. Bo Wang

- Constructed a standardized terahertz absorption-spectrum database by modeling first- and second-order statistical moments under varying experimental conditions.
- Developed a quadratic classification model based on maximum a posteriori estimation and shrinkage methods.
- Benchmarked the method against peak-based identification, conventional machine learning, and neural-network classifiers.
- **Publication:** Junwen Liao, Bo Wang, Zhiguo Wang, and Liguozhu. "Amino-acid classification based on terahertz absorption spectroscopy with Gaussian process and maximum likelihood." *Sensors and Actuators B: Chemical*, 2023. [Paper](#).

2021.09–2024.06

Applications of Terahertz Imaging in Medical Imaging

Advisor: Prof. Zhiguo Wang

- Established an imaging propagation model for terahertz waves in multilayer media.
- Studied model formulation and numerical solution strategies for terahertz-based medical imaging problems.

Selected Publications

1. **Junwen Liao***, Dihan Zheng*, Hui Zhang*, Linfeng Zhang, Mingxu Hu, and Chenglong Bao. "Fine-tuning AlphaFold with limited cryo-EM observations." *Communications Chemistry*, 2026.
2. **Junwen Liao**, Bo Wang, Zhiguo Wang, and Liguozhu. "Amino-acid classification based on terahertz absorption spectroscopy with Gaussian process and maximum likelihood." *Sensors and Actuators B: Chemical*, 2023.

* Equal contribution.

Teaching Experience

Fall 2024

Teaching Assistant, Linear Algebra

Tsinghua University

Assisted with course instruction and student support.

Awards and Honors

- Outstanding Graduate of Sichuan Province.
- Outstanding Student, Sichuan University.
- First-Class Comprehensive Scholarship, Sichuan University.
- Meritorious Winner, Mathematical Contest in Modeling (MCM/ICM).
- First Prize, Provincial Level, Chinese Mathematics Competitions.

Technical Background

Core areas

AI for science, computational imaging, inverse problems, statistical learning, generative modeling, protein structure prediction.

Methods

Differentiable forward modeling, cryo-EM particle supervision, deep learning for reconstruction, Gaussian-process-based classification, maximum a posteriori estimation.

Tools

Python, PyTorch, NumPy/SciPy, Git, LaTeX, and scientific visualization tools.

References

Prof. Chenglong Bao

Yau Mathematical Sciences Center, Tsinghua University

Ph.D. advisor

matbc.github.io/index.html

Prof. Zhiguo Wang

School of Mathematics, Sichuan University

Undergraduate advisor

zhiguo-wang-scu.github.io