# Yinkai Wang

Doctorate Candidate
Computer Science
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## Experience

**• Stanford University & AutoBio** *Stanford, CA*

*Visiting Scholar & Research Intern* June 2025 – August 2025

– Building VLM-based wet-lab video understanding, leveraging few-shot ICL and lightweight LoRA adapters.
– Designing a multi-agent workflow that turns captions into standardized, stepwise protocols.
– Establishing lean evaluation signals (faithfulness, coverage) with automated LLM-judge checks.
– Collaborating with Stanford and Nvidia researcher on AI-for-Science applications in agentic planning.

**• JD.com** *Dec 2021 - June 2022*

*Research Intern* Beijing, China

– Worked on text generation with a primary focus on creating text outputs that seamlessly blend with human-written content. This involved utilizing advanced algorithms and iterative training processes to refine the generated text, ensuring it met the desired quality standards.
– Engaged with the Unilm and LDA models to extract topics from customer reviews. This extracted information was then utilized to craft personalized written content for each customer, enhancing the user experience and ensuring content relevancy.

**• VDIG lab, Peking University** *Nov 2021 - Aug 2022*

*Researcher* Beijing

– Delved deep into object detection, a pivotal computer vision technique aimed at pinpointing instances of objects within images or videos. This research not only involved the application of established methodologies but also led to innovative outcomes, such as the introduction of the "objection" concept within object detection algorithms. This concept enhanced the interpretability of detection results.
– Leveraged the power of self-supervised learning (SSL) combined with transformer architectures to enhance object detection in images. This approach capitalized on unlabeled data, harnessing its potential to train models more effectively. The integration of transformer structures further improved the spatial understanding of the model, leading to more accurate and granular object detections.

**• ByteDance** *Apr 2021 - July 2021*

*Intern in DevEco* Beijing

– Concentrated on the foundational layer of Bytedance's host Android app, a critical component with intricate coupling relationships to a majority of Bytedance's applications. This involved understanding the app's architecture, and ensuring seamless integration and communication between the host app and other dependent apps.
– Pioneered the creation of a mock setting environment, a simulated platform tailored to facilitate QA testing. This innovative approach streamlined the testing process, reducing potential bottlenecks and significantly accelerating the publishing timeline, leading to more efficient release cycles.
– Championed the enhancement of the development environment, specifically catering to developers working on microapps within Bytedance. This initiative involved optimizing tools, workflows, and collaboration platforms, ensuring a productive and comfortable workspace that fostered creativity and efficiency.

## Selected Publications

**Large Language Model is Secretly a Protein Sequence Optimizer** [PDF]
*Accepted by LMRL ICLR 2025*
**Yinkai Wang**, Jiaxing He, Yuanqi Du, Xiaohui Chen, Jianan Canal Li, Li-Ping Liu, Xiaolin Xu, Soha Hassoun.

**MADGEN: Mass-Spec attends to De Novo Molecular generation** [PDF]
*Accepted by ICLR 2025*
**Yinkai Wang**, Xiaohui Chen, Liping Liu, Soha Hassoun

**Graph Generative Pre-trained Transformer** [PDF]
*Accepted by ICLR 2025 workshop (In submission to ICML)*
Xiaohui Chen, **Yinkai Wang**, Jiaxing He, Yuanqi Du, Xiaolin Xu, Soha Hassoun, Liping Liu.

**On Separate Normalization in Self-supervised Transformers** [PDF]
*Accepted by NeurIPS 2023*
Xiaohui Chen, **Yinkai Wang**, Yuanqi Du, Soha Hassoun, Liping Liu

**A Survey on Deep Graph Generation: Methods and Applications** [PDF]
*Accepted by LoG 2022*
**Yinkai Wang***, Yanqiao Zhu*, Yuanqi Du*, Jieyu Zhang, Qiang Liu, Shu Wu

**Small Molecule Generation via Disentangled Representation Learning** [PDF]
*Accepted by Bioinformatics 2022*
Yuanqi Du, Xiaojie Guo, **Yinkai Wang**, Amarda Shehu, Liang Zhao

**Multi-objective Deep Data Generation with Correlated Property Control** [PDF]
*Accepted by NeurIPS 2022*
Shiyu Wang, Xiaojie Guo, Xuanyang Lin, Bo Pan, Yuanqi Du, **Yinkai Wang**. (and 8 others)

**Deep Latent-Variable Models for Controllable Molecule Generation** [PDF]
*Accepted by BIBM 2021*
Yuanqi Du, **Yinkai Wang**, Fardina Alam, Yuanjie Lu, Xiaojie Guo, Liang Zhao,Amarda Shehu.

**Dataset Geography: Mapping Language Data to Language Users** [PDF]
*Accepted by ACL 2022*
Fahim Faisal, **Yinkai Wang**, Antonis Anastasopoulos

## Research Statement

My research focuses on AI for Science, with an emphasis on generative modeling and cross-modal learning for molecular discovery. I develop deep graph generative models, diffusion-based frameworks, and cross-attention mechanisms that bridge molecular structures with experimental data such as tandem mass spectra. This includes work on MADGEN (ICLR 2025), which conditions molecular generation on spectral peaks, and G2PT, a pre-trained graph transformer designed for broad molecular generation tasks. Earlier contributions include disentangled representation learning for small molecules, a widely cited survey on deep graph generation, and advances in normalization methods for self-supervised transformers. Together, these efforts build methodological foundations for reliable and controllable molecular generation.

More recently, I have extended my research toward multimodal and agentic AI systems that integrate molecular data with laboratory workflows. At Stanford, I developed pipelines where visionlanguage models process wet-lab videos into stepwise experimental protocols, leveraging few-shot prompting, LoRA adapters, and multi-agent reasoning. Looking forward, my goal is to design foundation models for molecular science that unify diverse modalitiesgraphs, spectra, proteins, and laboratory observationsinto a coherent reasoning and generation framework. These systems will enable scalable hypothesis generation, molecular and protein design, and automated experimental planning, accelerating discovery in chemistry and biology.

## Education

- **Ph.D in Computer Science** *2022-Present*
  *Tufts University, United States*
- **Master in Computer Science** *2022-2024*
  *Tufts University, United States*
- **Bachloar in Computer Science** *2018-2021*
  *George Mason University, United States*
- **Bachloar in Computer Science** *2017-2022*
  *Huaqiao University, United States*

## Selected Academic Services

- **ICML reviewer** *2024-present*
- **ICLR reviewer** *2024-present*
- **NeurIPS reviewer** *2023-present*
- **NeurIPS Datasets and Benchmarks reviewer** *2022-present*
- **AAAI reviewer** *2022-present*