DAC WorkGroup on Scientific AI Agents
University of Notre Dame

Meng Jiang

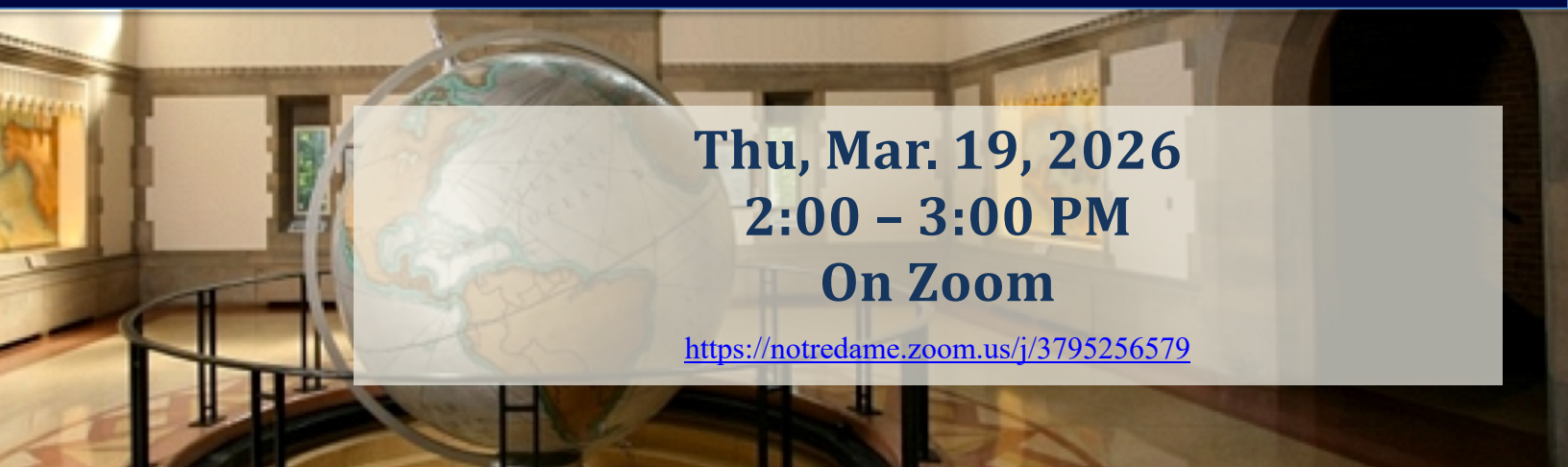
University of Notre Dame

Multimodal Machine Learning in Molecular AI

Scientific discovery increasingly demands AI systems that can reason, generate, and design across multiple modalities, ranging from text and molecular graphs to reaction sequences and material properties. In this talk, I present recent advances in multimodal machine learning, as a foundation of tools and models for building molecular AI agents capable of understanding, predicting, and designing polymers and small molecules.

I first present repetition-invariant graph learning and multimodal graph-sequence fusion to improve molecular and polymer property prediction, yielding more robust, interpretable representations and stronger performance across materials and drug benchmarks. I then introduce data-centric learning with rationalization-based augmentation and Graph Diffusion Transformers to enable controllable, multi-conditional molecular generation and inverse design. Finally, I present multimodal large language models that coherently generate molecules, properties, and retrosynthetic plans, demonstrating improved controllability, expert-preferred designs, and in-context molecular optimization.

Together, these advances outline a pathway toward general-purpose scientific AI agents that integrate multimodal reasoning, generative modeling, and domain knowledge to accelerate materials discovery and drug design while lowering the barrier to molecular AI through tools such as Torch-Molecule.



Thu, Mar. 19, 2026
2:00 – 3:00 PM
On Zoom

https://notredame.zoom.us/j/3795256579