

CS 6824: AI-powered Molecular Modeling

This course will survey the emerging field of computational modeling of molecular structures driven by advances in artificial intelligence (AI), with an emphasis on predictive modeling. We will investigate relevant issues from interdisciplinary perspectives of macromolecular modeling and machine learning.

Topics will include:

- Deep learning-based molecular modeling
- Language modeling of molecular sequences
- Macromolecular geometry learning and representation
- End-to-end learning: from sequence to structures
- AI-driven conformational sampling and scoring
- Human-in-the-loop molecular modeling

The course will emphasize readings in the scientific literature and novel projects.