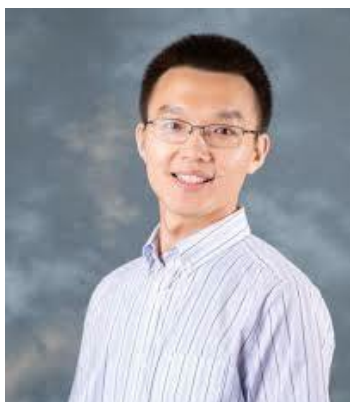


XINQIANG DING

Assistant Professor of Chemistry

Tufts University



Thursday, November 6th

10:30 AM - 11:30AM

Steele 006

“Advancing Free Energy Methods with Generative Models”

Abstract: Generative machine learning models are becoming increasingly powerful tools in modeling high dimensional probability distributions, such as distributions of images, languages, and molecules. In this talk, I will discuss how we can leverage these generative models to improve free energy calculations by combining them with established statistical mechanics techniques. I will first provide a brief overview of traditional free energy methods, highlighting their strengths and limitations. Next, I will show how generative models can be integrated into these methods to enhance computational efficiency. Specifically, I will focus on using the method for estimating binding free energies of molecular systems, demonstrating how generative models can help dramatically reduce the number of required simulations while maintaining accuracy.

Bio: I am an assistant professor in the Department of Chemistry at Tufts University. My general research interest is developing new computational methods to study complex molecular systems. I received my Ph.D. from the University of Michigan and completed my postdoctoral training at MIT. My current research focuses on leveraging machine learning techniques, particularly generative models, to improve molecular simulations and free energy calculations. I received the Young Investigator Award from the American Chemical Society when I was a postdoc and recently received an NIH MIRA award to support my independent research program.