Abstract: Genome sequencing and high-throughput techniques have generated vast amounts of diverse biological and clinical data. However, these sets of data have not yet been fully explored to improve the effectiveness and efficiency of drug discovery. Many diseases such as cancers, Alzheimer's disease, and emerging COVID-19 do not have safe and effective therapeutics. There is hyperbole that Artificial Intelligence would accelerate drug discovery. However, the successful application of AI to biomedicine faces many technical and fundamental challenges which have not been fully appreciated. In this talk, I will present our recent work in developing data-driven framework for the multi-scale modeling of biological system using noisy, biased, and heterogeneous data. Specifically, I will introduce several new deep learning algorithms that are developed in my lab for addressing challenges in drug discovery and precision medicine. They include graph attention network for graph representation, self-supervised learning for unlabeled or noisy data, and multi-layered network model for data integration. Furthermore, I will highlight the importance in integrating mechanism-based modeling and deep learning for knowledge discovery.

Biography: Dr. Lei Xie joined CUNY in 2011. He is currently a professor in Computer Science at Hunter College, and affiliated with Ph.D. program at Computer Science, Biochemistry, and Biology at the Graduate Center. He is also an Adjunct Professor in Neuroscience at Weill Cornell Medicine, Cornell University. His research focuses on developing new methods in machine learning, informatics, systems biology, and biophysics for multi-scale modeling of causal genotype-phenotype associations and drug actions, and applying them to drug discovery and precision medicine. From 2001 to 2011, he was a principle scientist at San Diego Supercomputer Center (SDSC), research scientist in pharmaceutical company Hoffmann-La Roche, and biotechnology start-up Eidogen. He was trained in Computational Biology and Biophysics as a postdoctoral fellow at Columbia University and Howard Hughes Medical Institute from 2000 to 2001. He obtained his Ph.D. in Medicinal Chemistry and M.S. in Computer Science from Rutgers University, and B.S. in Polymer Physics from University of Science and Technology of China.