Graph Computing for Quantum Chemistry and Physics

Shuiwang Ji
Professor and Presidential Impact Fellow
Department of Computer Science & Engineering
Texas A&M University

ABSTRACT: While classic physics is concerned with objects in the macro world, quantum physics and chemistry deal with particles at the atomic scale. In this talk, I will present our work on using deep learning and graph computing to accelerate scientific discoveries in the quantum field. Specifically, we consider representation learning of 3D molecular graphs in which each atom is associated with a spatial position in 3D. This is an under-explored area of research, and a principled neural message passing framework is currently lacking. We propose the spherical message passing as a novel and powerful scheme for 3D molecular learning. Based on 3D information representation in quantum physics, we develop the SphereNet for 3D molecular learning. In addition to predictive tasks, we consider the problem of generating 3D molecular geometries. We propose G-SphereNet as a novel autoregressive flow model for generating 3D molecular geometries. G-SphereNet employs a flexible sequential generation scheme by placing atoms in 3D space step-by-step. Experimental results show that SphereNet and G-SphereNet outperforms prior methods on predictive and generative tasks. Both SphereNet and G-SphereNet have been accepted to ICLR 2022.