

Graph Computing for Quantum Chemistry and Physics

Date: 23 March 2022 (Wednesday)

Time: 10:00am - 11:00am

Seminar link: <https://cityu.zoom.us/j/98664636998>



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.



Prof Shuiwang Ji GUEST SPEAKER'S PROFILE

Prof Shuiwang Ji is currently a Professor and Presidential Impact Fellow in the Department of Computer Science & Engineering, Texas A&M University. He received the Ph.D. degree in Computer Science from Arizona State University in 2010. His research interests include artificial intelligence, machine learning, and quantum information science. Prof Ji received the National Science Foundation CAREER Award in 2014. Currently, he serves as an Associate Editor for IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI), ACM Transactions on Knowledge Discovery from Data (TKDD), and ACM Computing Surveys (CSUR). He regularly serves as an Area Chair for AAAI Conference on Artificial Intelligence (AAAI), International Conference on Learning Representations (ICLR), International Conference on Machine Learning (ICML), International Joint Conference on Artificial Intelligence (IJCAI), ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), and Annual Conference on Neural Information Processing Systems (NeurIPS). Prof Ji is a Fellow of AIMBE, a Distinguished Member of ACM, and a Senior Member of IEEE.