Chez Pierre

Presents ...

Monday, September 16, 2024

12:00 pm - 1:00 pm

Duboc Room – 4-331

Chez Pierre Seminar

Mingda Li (NSE, MIT)

"Exploring Potential Roles of Machine Learning in Quantum Materials Research".

In recent years, machine learning in chemistry and materials science has seen success, but quantum materials face unique challenges: scarce data, high dimensionality and computational costs, and elusive experimental signatures with unreliable ground truth. In this Chez-Pierre Seminar, we discuss our efforts to support quantum materials study with machine learning. When high data volumes are feasible, machine learning can predict properties, such as using a convolutional neural network to classify band topology based on X-ray absorption signals [1]. We also demonstrate an auto encoder-based protocol to study the magnetic proximity effect with polarized neutron reflectometry [2]. In low data volume scenarios, incorporating symmetry into neural networks reduces needed data. Using the symmetry-aware neural networks, we predict phonon density-of-states [3], dielectric functions and quantum weight [4] from crystal structures. Machine learning without data can use differential equations as constraints [5]. For high output dimensions, we introduce graph neural networks with virtual nodes to predict phonon dispersion relations efficiently [6]. To tackle unreliable ground truth, we use machine learning to distinguish Majorana zero modes in scanning tunneling spectroscopy [7]. Our SCIGEN generates crystal structures under geometrical constraints, producing materials with potential geometrical frustration and over 50% passing DFT stability checks for quantum spin liquid candidates [8]. Despite progress, machine learning for quantum materials is still in its infancy. We must address out-of-distribution problems to generate genuinely new features and improve accuracy for complex quantum systems and phase diagrams.

[1] NA, ML, “Machine learning spectral indicators of topology,” Advanced Materials 34, 202204113 (2022).

[2] NA, ML, "Elucidating proximity magnetism through polarized neutron reflectometry and machine learning," Applied Physics Review 9, 011421 (2022).

[3] ZC, ML, “Direct prediction of phonon density of states with Euclidean neural networks,” Advanced Science 8, 2004214 (2021).

[4] NH, ML, “Ensemble-Embedding Graph Neural Network for Direct Prediction of Optical Spectra from Crystal Structure,” arXiv:2406.16654.

[5] ZC, ML, "Panoramic mapping of phonon transport from ultrafast electron diffraction and machine learning," Advanced Materials 35, 2206997 (2023).

[6] RO, AC, ML, "Virtual Node Graph Neural Network for Full Phonon Prediction," DOI:10.1038/s43588-024-00661-0, Nature Computational Science (2024).

[7] MC, ML, “Machine Learning Detection of Majorana Zero Modes from Zero Bias Peak Measurements,” Matter 7, 2507 (2024).

[8] RO, ML, "Structural Constraint Integration in Generative Model for Discovery of Quantum Material Candidates," arXiv:2407.04557.