Topological Kohn anomaly and machine-learning augmented phonon DOS prediction

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Abstract: Inelastic X-ray scattering (IXS) at meV scale represents a powerful experimental technique that studies materials elementary excitation with ultrahigh resolution. In this presentation, I will introduce how quantum field theory and machine learning can aid IXS discoveries of quantum materials. In one example, quantum field-theoretical calculations predicted the presence of a new class of Kohn anomaly in topological Weyl semimetal materials, that the electronic topology leaves hallmark phonon softening at specific points in Brillouin zone [1]. This theoretical prediction enables a direct experimental probing of Kohn anomaly with IXS, with ~1% error comparing with theory. In another example, using the symmetry-preserved neural networks, we have built a machine-learning-based predictor that can output phonon density-of-states in crystalline solid by directly using atomic structure files. The approach reaches ab initio accuracy for 80% of materials with significantly lowered computational cost, especially for alloys [2]. I will conclude by showing the increasingly important roles theory and machine learning may play to study quantum materials through the probe of IXS [3].

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[2] Z. Chen†, N. Andrejevic†, T. Smidt†, Z. Ding, Y-T Chi, Q. Nguyen, A. Alatas, J. Kong and M. Li*, "Direct prediction of phonon density of states with Euclidean neural networks", DOI:10.1002/advs.202004214, Advanced Science (2021). (†Equal contribution)

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