Characterizing Quantum Materials with Integrated Experiments and Machine Learning

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The past few years have witnessed booming research in machine learning in chemistry and materials sciences. New pharmaceutical molecules and new energy materials have been identified by machine learning, leading to a paradigm shift in research and industry. Quantum materials, on the other hand, despite constant new reports of using machine learning, have experienced significant challenges due to the complex interplay between the charge, spin, orbital, and lattice degrees of freedom, and the often-met out-of-distribution (OOD) problem.

In this ICTP workshop, we introduce our recent efforts in connecting machine learning to various quantum materials, particularly when connected with various experimental techniques. For topological materials with band topology, since "topology" itself is not measurable, seeking the experimental manifestation becomes critical. We introduce our recent effort, to use machine learning to improve interfacial magnetism resolution [1], and to detect band topology with over 90% accuracy from simple spectra [2]. For collective excitations of phonons, measurable by inelastic scattering, we show how 3D symmetry can be encoded into a neural network that could lead to efficient property predictions [3], and beyond that how to encode the Brillouin zone into real-space graph neural network to predict complex materials [4]. We present our most recent work on machine learning to classify Majorana bound state from tunneling conductance data, even the OOD problem is severe [5]. We conclude by presenting a few more examples showing the increasingly important role machine learning may play in a variety of quantum many-body and scattering experiments even with scarcity of data and challenges in computation.

[1] NA, ZC, ML, Appl. Phys. Rev. **9**, 011421 (2022)
[2] NA, ML Advanced Materials **34**, 202204113 (2022)
[3] ZC, NA, ML. Advanced Science **8**, 2004214 (2021), ZC, XS, ML, Advanced Materials 35, 2206997 (2023)
[4] RO, AC, ML, arXiv:2301.02197 (2023), In production, *Nature Computational Science* (2024).
[5] MC, RO, AC, ML, arXiv:2310.18439 (2023), In Production, *Matter* (Cell Press) (2024).

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