Machine learning approaches in Property Analysis and Simulation Package for materials (PASP)

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Abstract: We have developed a software package, namely, PASP (Property Analysis and Simulation Package for materials), to analyze the structural, electronic, magnetic, and thermodynamic properties of complex condensed matter systems. Our package integrates several functionalities including group theory analysis, global structure searching methods, tight-binding approach, effective Hamiltonian methods, Monte Carlo simulation, spin-lattice dynamic simulation methods, and machine learning approaches. In this talk, I will mainly focus on the implemented machine learning approaches in PASP. In particular, I will discuss our newly developed machine learning potential approach for magnetic systems, the transferable equivariant graph neural networks for the electronic Hamiltonians of molecules and solids, and the universal machine learning electronic Hamiltonian for any materials. The applications of these machine learning approaches to two-dimensional magnets, electron phonon coupling related phenomena, and high-throughput search of new functional materials will be presented as well.