Computational Discovery of Novel Materials: From DFT to Machine Learning

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Abstract:

To reduce design of experiments costs, as the first step, to predict new materials (especially 2Dmaterials) different theoretical approaches, especially those are based on the DFT are employed. On the other words, theory can provide guidance to the experiments, and in many cases give deeper insights and offer promising candidates for the experimental peers to explore. To find a new material, in a systematic investigation, prior to properties investigations, people typically conduct structural search and optimization, confirm thermodynamic stability (by computing the cohesive energies), evaluate kinetic stability (by computing phonon dispersion, make sure that the material is at least a local minimum), and check Thermal stability by first principles MD simulations. However, each of these steps requires massive amounts of computation and costs long times. Therefore, both theoretical and experimental screening methods often consume tremendous time and computational or/and experimental resources. Thus, it is imperative to develop a new method of accelerating the discovery and design process for novel materials. Considering the issue, the advantages of Machine Learning (ML) is proposed for the evaluation and screening of new materials. In this talk, by presenting a number of my contributions in the field of DFT based prediction of novel materials and materials properties investigation, the necessity of using ML scheme for conducting more efficient project in the field of novel materials discovery will be discussed.
Key Words: Materials Discovery, First principles prediction, DFT, Machine Learning