Ab Initio and Machine Learning Methods for (Non-)Adiabatic Molecular Dynamics of Materials

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Adiabatic and non-adiabatic molecular dynamics are powerful approaches for modeling the behavior of electrons and atoms in materials, which determines the performance of many modern technologies such as batteries and solar cells. The simulations usually rely on solving the Schrödinger equation at the ab initio level, which is accurate but costly for large systems, hindering the investigation of realistic conditions. In recent years, machine learning has emerged as a gamechanger to significantly accelerate many calculations. This breakthrough is expected to enable the modeling of many large-scale processes which are unavailable before. This lecture will briefly review the ab initio methods in material studies and introduce some recently developed machine learning interatomic potentials and Hamiltonian models. Some applications will be provided as well. We anticipate that the lecture can show the potential of machine learning in advancing the modern computational materials science.

Bibliography

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