DFT-Machine Learning Approach for Organic Electrode Materials for Li-ion Battery

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In this talk, the first-principles density functional theory modeling of redox properties of various organic materials is presented. First, the contribution of electron affinity of molecules and solvation to redox potential are discussed from density functional theory (DFT) calculations. Second, the relationship of redox potential with the design of molecular structure. It is found that aromaticity and electron-withdrawing functional groups can be used to tune the redox potential. Especially, the variation of redox potential as a function of Li association is discussed. From this DFT study, it is concluded that the redox potential can be tuned by designing molecular structure. Next, machine learning models such as artificial neural network and kernel ridge regression are developed using the DFT results. Through this study, the redox characteristics of organic materials are systematically investigated using the first-principles DFT modeling, and then utilized via machine learning methods for high-throughput screening process.