First-principles calculations; a powerful tool to study materials from physics to materials science

Density functional theory (DFT) is a popular quantum method for fundamental physics and industrial applications. Using first-principles calculations based on DFT, when we know the information of a crystal structure, the properties of the crystal can be obtained without any empirical parameters. It makes DFT be a powerful tool in modern solid-state physics and computational materials science. As examples, in this talk, I will present my recent work on high *T*c superconductivity and battery cathode materials. For copper-based superconductors, the maximum superconducting transition temperature *T*c,max of different families measured from experiment can vary from 38 K in La2CuO4 to 135 K in HgBa2Ca2Cu3O8 at the optimal hole doping concentration. We demonstrate, using first-principles calculations, a new trend suggesting that the cuprates with stronger out-of-CuO2-plane chemical bonding between the apical anion (O, Cl) and apical cation (e.g., La, Hg, Bi, Tl) are generally correlated with higher *T*c,max in experiments. We then show the underlying fundamental phenomena of coupled apical charge flux and lattice dynamics when the apical oxygen oscillates vertically. I will introduce research on battery materials as the second part of my talk. Recently, Cu element has been introduced into layered sodium transition metal oxides (NaxTMO2) as cathode materials for sodium-ion batteries to engineer rate and cycling performance. I will introduce our studies on P2-type NaxTMO2 cathodes for a better high voltage performance combining the first principle calculations and experiments. Especially, we focus on Cu element and study the unique role provided by Cu in NaxTMO2. We observed the P2 to O2-like phase transition of MnFeCu-based materials upon charging and studied its influence on battery performance. We show that different Na diffusivity and site preference in the high voltage phase contribute to the difference in the electrochemical performances of these cathode materials.