Electronic Structure of Energy-Related Materials with Many-Body Effects: From Battery Cathodes to Rare-Earth Magnetic Compounds

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Abstract

The rapidly developing society nowadays necessitates the utilization and investigation of energy-related materials. These materials encompass a wide spectrum, ranging from battery materials intended for powering electric units and energy storage, to rare earth (RE)-based intermetallic systems for permanent magnets and spintronic applications. Comprehension of the electronic structure of these materials has the potential to reveal new physics. Furthermore, such understanding serves as a foundation for the design of novel systems with desired properties.

For many weakly correlated systems, the single-particle picture has historically been proven to be sufficient and successful in describing their physical properties of interest. However, in many cases, the many-body effects are non-negligible, for instance, when treating the highly correlated nature of 4f electrons in RE elements and their compounds. In this presentation, I will first demonstrate how to understand the evolution of the physicochemical bulk properties during the Li deintercalation (charging) process in $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ cathode battery material, via a combination of X-ray photoelectron spectroscopy (XPS), density functional theory plus dynamical mean-field theory (DFT+DMFT) calculations, and charge transfer multiplet (CTM) model simulations. Furthermore, the many-body effects have been considered in order to address the mixed-valence nature of Ce in $CeCo_5$-based compounds and their intrinsic magnetic properties. Moreover, the mechanism underlying bulk perpendicular magnetic anisotropy (PMA) in amorphous TbCo films has been elucidated by constructing a many-body Hamiltonian of Tb atoms situated under various local crystalline environments. A particularly intriguing aspect of this phenomenon is the observation that the perturbation of local crystalline environments through hydrogenation can readily alter the easy magnetization direction.