Infiltration of Single-Ion Magnets into Metal-Organic Frameworks for Controlled Nanostructuration: Translation of Density Functional Theory to the Experiment

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Ultra high-density data storage materials are vital components for next-generation computing. Single-ion magnets (SIMs) have received significant attention in recent years for their unique magnetic properties. SIMs exhibit magnetic hysteresis at low temperatures and can be used in spintronics for switching from total spin up to spin down on a molecular level where each molecule serves as a magnetic bit of information. It has been proposed that these properties will allow SIMs to be used for the design of revolutionary high-density information storage devices. However, before their practical applications can be explored, it is necessary to isolate and organize the SIM molecules from one another to allow for rational read and write processes. Metal-organic frameworks (MOFs), porous, crystalline materials composed of metal nodes and organic ligands, have been proposed as host matrix for SIMs. The MOFs' large accessible pores enable the effective immobilization of SIMs while protecting their desired unique properties of magnetic bistability. In this presentation, we focus on the infiltration of SIMs into MOFs as a translation of solid-state density functional theory to the experiment to comprehend given structure-property relationships.