

Itinerant ferromagnetism in a mixed-valent metal-organic framework: A DFT Perspective

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Materials that display favorable magnetic ordering with other desirable physical properties have the potential to revolutionize active areas of research such as spintronics, quantum sensing, low-density magnets, and magnetic gas separations. As such, efforts to design multifunctional magnetic materials have transitioned beyond traditional solid-state compounds to metal-organic solids. Among these solids, metal-organic framework (MOF) materials bear structures that offer intrinsic porosity and tunability of chemical and electronic structures, which are attractive physical properties for these applications. Here, we investigate the phenomenon of itinerant ferromagnetism in a mixed-valence chromium (II/III) triazolate material by the use of spin-polarized Density Functional Theory (DFT). We aim to understand, characterize, and utilize MOFs as magnetic materials.

