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Structural, chemical bonding, electronic and magnetic properties of KMF_3 (M = Mn, Fe, Co, Ni) compounds

Abstract

KMF_3 (M = Mn, Fe, Co, Ni) compounds crystallize in the cubic perovskite structure with space group *Pm3m* (#221) at ambient conditions. Structural, chemical bonding, electronic and magnetic properties of these compounds are investigated using the full-potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT). The calculated structural parameters agree well with the experimental measurements. From the elastic properties, it is inferred that these compounds are elastically stable. Moreover, $KMnF_3$ is found to be ductile in nature while the remaining compounds are brittle. The results of the electronic band structure show that $KMnF_3$ and $KNiF_3$ are indirect band gap semiconductors in both spin channels, while $KFeF_3$ and $KCoF_3$ are half metallic, being semiconductors with majority spin channel and metals with spin minority channel. The bonding behavior of the studied compounds is expressed as a combination of covalent–ionic behavior. The magnetic study reveals the ferromagnetic behavior for these compounds. The half metallicity and the ferromagnetic behavior favor these compounds for spintronic applications.

Keywords; Fluoroperovskites, DFT, Electronic properties, Magnetic properties