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Electronic, Structure and Magnetic Properties of KXF3(X= Fe, Co, Mn, V) from Ab Initio Calculations

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Abstract : We have performed first-principle calculations of the structural, electronic and magnetic properties of KFeF3, KCoF3, KMnF3, KVF3, using full-potential linearized augmented plane-wave (FP-LAPW) scheme within GGA. Features such as the lattice constant, bulk modulus and its pressure derivative are reported. Also, we have presented our results of the band structure and the density of states. The magnetic moments of KFeF3, KCoF3, KMnF3, KVF3 compounds are in most came from the exchange-splitting of X-3d orbital.

Keywords : Ab initio calculations, electronic structure, magnetic materials
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