Poster Presentation

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Ab-initio study of the orthorhombic NdMnO3 perovskite

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We investigate the structural, electronic and magnetic properties of the orthorhombic Perovskite oxyde NdMnO3 through density-functional-theory (DFT) calculations using both generalized gradient approximation GGA+U, where U is on-site Coulomb interaction correction. The electronic band structure, the partial and total density of states (DOS) and the magnetic moment are determined. The results show a half-metallic ferromagnetic ground state for the orthorhombic NdMnO3.

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