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AB-INITIO STUDY OF STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF $RbFeO_3$AND $CsFeO_3$ MATERIALS

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Abstract **–**A density functional theory DFT was applied to calculate structural, electronic and magnetic properties of Alkali iron perovskites. Gradient generalized approximations GGA-PBE and GGA-WC within DFT were implemented in CASTEP code (Cambridge Serial Total Energy Package) to conduct our calculations. Ultra-soft plane wave pseudo-potentials were used to solve Cohen-Sham equations. For the two materials $RbFeO_3$ and $CsFeO_3$, we found cubic and ferromagnetic ground states. Results indicate also lattice parameters between 3,80A° and 3,96A° and magnetic moments between 4,45 μ_B and 4,57μ_B. Band structures showed that both materials were conductors. This work prospect that the two compounds candidate to utilize in spintronics technology.

Keywords –DFT, CASTEP, $RbFeO_3$, $CsFeO_3$, Magnetic Moments.