Structural, electronic and magnetic properties RbRuO₄; A theoretical study

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Abstract – Ruthenate oxide materials are significant compounds in magnetic technologies because they have an important element in transition metals. Herein we make a density functional theory (DFT) investigation to study the structural, electronic, and magnetic properties of rubidium ruthenium oxide RbRuO₄. Gradient generalized approximation, GGA-PBE, and GGA-WC within Cohen-Sham equations were implemented in the CASTEP code and used in our calculations. Plane-wave pseudo potential method was used to simplify the electrons-Ions interactions. Results showed a ferromagnetic ground state of the material studied here. For the structural properties, RbRuO₄ crystallizes in the orthorhombic structure (Pnma space group). In calculations of lattice parameters, we found a volume of primitive cells between 477 Å³ and 482 Å³ and bulk modulus between 82,12 GPa and 86,65 GPa. Finally, the band structure energies showed that RbRuO₄ had a metallic nature.

Keywords – RbRuO₄ ; DFT ; Ferromagnetic ; Metallic ; Orthorhombic Structure