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Structural, electronic and magnetic properties $RbRuO_4$; A theoretical study

Ahmed Memdouh Younsi[1,2,*], Abdelaziz Rabehi[2]

[1]*University of Biskra, Laboratory of Physics of Photonics and Multifunctional Nanomaterials, BP 145, RP, 07000 Biskra, Algeria.*

[2]*Materials Science and Informatics Laboratory, University of ZianeAchourDjelfa, Post Office Box 3117, 17000 Djelfa, Algeria.*

[*]*(ahmed.younsi@univ-biskra.dz) Email of the corresponding author*

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, $RbRuO_4$ crystallizes in the orthorhombic structure (Pnma space group). In calculations of lattice parameters, we found a volume of primitive cells between 477 A°3 and 482 A°3 and bulk modulus between 82,12 GPa and 86,65 GPa. Finally, the band structure energies showed that $RbRuO_4$ had a metallic nature.

Keywords – $Rbruo_4$; DFT ; Ferromagnetic ; Metallic ; Orthorhombic Structure