EuroSciCon

EuroSciCon Conference on

Advanced Nanotechnology

April 18-19, 2019
Paris, France

Nano Res Appl 2019, Volume:5
DOI: 10.21767/2471-9838-C2-034

OPTOELECTRONIC, MAGNETIC AND STRUCTURAL PROPERTIES OF DOUBLE PEROVSKITE MATERIALS AFFECTING IN NANOTECHNOLOGY FIELD

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In this paper, we have investigated the structural, electronic, magnetic and optical properties of cubic double perovskite Sr_2CrZrO_6 using the full-potential linearized augmented plane wave method (FP-LAPW), based on the density functional theory (DFT) as implemented in the WIEN2K code. The exchange correlation potentials is treated by the generalized gradient approximation (GGA), GGA+U where U is on-site coulomb interaction correction as well as modified Becke-Johnson (mBJ) which have been used to correct the potential. Calculations were performed with the Birch-Murnaghan approach to determine the equilibrium phase, lattice, bulk modulus and its pressure derivative. The results display a half-metallic ferromagnetic ground state for the cubic double perovskite Sr_2CrZrO_6 compound due to the strong correlation effect of transition metal Cr(3d-t2g) states with the integer value of the total magnetic moment. Furthermore, we found a direct gap (Γ-Γ) around the Fermi level, making this material Sr_2CrZrO_6 a competent candidate for optoelectronic and spintronic applications in the future of Nanotechnology.

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