World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:17, No:08, 2023

An ab initioStudy of the Structural, Elastic, Electronic, and Optical Properties of the Perovskite ScRhO3

Authors : L. Foudia, K. Haddadi, M. Reffas

Abstract : First principles study of structural, elastic, electronic and optical properties of the monoclinic perovskite type $ScRhO_3$ has been reported using the pseudo-potential plane wave method within the local density approximation. The calculated lattice parameters, including the lattice constants and angle β, are in excellent agreement with the available experimental data, which proving the reliability of the chosen theoretical approach. Pressure dependence up to 20 GPa of the single crystal and polycrystalline elastic constants has been investigated in details using the strain-stress approach. The mechanical stability, ductility, average elastic wave velocity, Debye temperature and elastic anisotropy were also assessed. Electronic band structure and density of states (DOS) demonstrated its semiconducting nature showing a direct band gap of 1.38 eV. Furthermore, several optical properties, such as absorption coefficient, reflectivity, refractive index, dielectric function, optical conductivity and electron energy loss function, have been calculated for radiation up to 40 eV.

Keywords : ab-initio, perovskite, DFT, band gap
Conference Title : ICSPN 2023 : International Conference on Structure Physics and Nanomaterials
Conference Location : Paris, France
Conference Dates : August 24-25, 2023