World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

Electronic and Optical Properties of YNi4Si-Type DyNi4Si Compound: A Full Potential Study

Authors : Dinesh Kumar Maurya, Sapan Mohan Saini

Abstract : A theoretical formalism to calculate the structural, electronic and optical properties of orthorhombic crystals from first principle calculations is described. This is applied first time to new YNi4Si-type DyNi4Si compound. Calculations are performed using full-potential augmented plane wave (FPLAPW) method in the framework of density functional theory (DFT). The Coulomb corrected local-spin density approximation (LSDA+U) in the self-interaction correction (SIC) has been used for exchange-correlation potential. Our optimized results of lattice parameters show good agreement to the previously reported experimental study. Analysis of the calculated band structure of DyNi4Si compound demonstrates their metallic character. We found Ni-3d states mainly contribute to density of states from -5.0 eV to the Fermi level while the Dy-f states peak stands tall in comparison to the small contributions made by the Ni-d and R-d states above Fermi level, which is consistent with experiment, in DNi4Si compound. Our calculated optical conductivity compares well with the experimental data and the results are analyzed in the light of band-to-band transitions. We also report the frequency-dependent refractive index n(ω) and the extinction coefficient k(ω) of the compound.

Keywords : band structure, density of states, optical properties, LSDA+U approximation, YNi4Si- type DyNi4Si compound
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020