

## Electronic and Optical Properties of YNi<sub>4</sub>Si-Type DyNi<sub>4</sub>Si Compound: A Full Potential Study

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**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 YNi<sub>4</sub>Si-type DyNi<sub>4</sub>Si compound. Calculations are performed using full-potential augmented plane wave (FP-LAPW) 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 DyNi<sub>4</sub>Si 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 DNi<sub>4</sub>Si 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  $n(\omega)$  and the extinction coefficient  $k(\omega)$  of the compound.

**Keywords :** band structure, density of states, optical properties, LSDA+U approximation, YNi<sub>4</sub>Si- type DyNi<sub>4</sub>Si compound

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