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First Principle Study of Electronic and Optical Properties of YNi_4Si-Type $HoNi_4Si$ Compound

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Abstract : We investigate theoretically the electronic and optical properties of YNi_4Si-type $HoNi_4Si$ compound from first principle calculations. Calculations are performed using full-potential augmented plane wave (FPLAPW) method in the frame work 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. Analysis of the calculated band structure of $HoNi_4Si$ 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 Ho-f states peak stands tall in comparison to the small contributions made by the Ni-d and Ho-d states above Fermi level, which is consistent with experiment, in HoNi4Si compound. Our calculated optical conductivity compares well with the experimental data and the results are analyzed in the light of band to band transitions.

Keywords : electronic properties, density of states, optical properties, LSDA+U approximation, YNi_4Si-type HoNi4Si compound
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