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Electronic Structure and Optical Properties of YNi_4Si-Type $GdNi_5$: A Coulomb Corrected Local-Spin Density Approximation Study

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Abstract : In this work, we report the calculations on the electronic and optical properties of YNi_4Si-type $GdNi_5$ compound. Calculations are performed using the 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. Spin polarised calculations of band structure show that several bands cross the Fermi level (EF) reflect the metallic character. Analysis of density of states (DOS) demonstrates that spin up Gd-f states lie around 7.5 eV below EF and spin down Gd-f lie around 4.5 eV above EF. We found Ni-3d states mainly contribute to DOS from -5.0 eV to the EF. Our calculated results of optical conductivity agree well with the experimental data.

Keywords : electronic structure, optical properties, FPLAPW method, YNi_4Si-type $GdNi_5$
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