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First Principls Study of Structural, Electronic, Magnetic and Optical Properties of $SiNi_2O_4$ Spinel Oxide

Authors : Karkour Selma

Abstract : We conducted first principles full potential calculations using the Wien2k code to explore the structural, electronic, magnetic, and optical properties of $SiNi_2O_4$, a cubic normal spinel oxide. Our calculations, based on the GGA-PBEsol of the generalized gradient approximation, revealed several key findings. The spinel oxides exhibited a stable cubic structure in the ferromagnetic phase and showed 100% spin polarization. We determined the equilibrium lattice constant and internal parameter values. In terms of the electronic properties, we observed a direct bandgap of 2.68 eV for the spin-up configuration, while the spin-down configuration exhibited an indirect bandgap of 0.82 eV. Additionally, we calculated the total density of states and partial densities for each atom, finding a magnetic moment spin density of states of 8.0 μB per formula unit. The optical properties have been calculated. The real, $\varepsilon_1(\omega)$ and the imaginary, $\varepsilon_2(\omega)$ parts of the complex dielectric constants, refractivity, reflection and energy loss when light scattered from the material. The absorption region spanned from 1.5 eV to 14 eV, with significant intensity. The calculated results confirm the suitability of this material for optical and spintronic devices application.

Keywords : DFT, spintronic, GGA, spinel
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