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Electronic Structure of $NiFe_2O_4$ using screened Hybrid Functionals HUNTER SIMS, MINT Center and Dept. of Physics, University of Alabama, DIPANJAN MAZUMDAR, MINT Center, University of Alabama, SANJOY SARKER, MINT Center and Dept. of Physics, University of Alabama, ARUNAVA GUPTA, MINT Center, University of Alabama, QI SUN, JAN MUSFELDT, Department of Chemistry, University of Tennessee — As an insulating ferrimagnet with a high Curie temperature, $NiFe_2O_4$ (NFO) may be a promising candidate for future spin-based applications. Recent demonstration of spin-Seeback effect in magnetic insulators indicates that important new phenomena may be discovered in such materials. Unfortunately, density functional theory cannot give a full account of its properties; most notably, LDA calculations find it to be metallic. LDA+U yields an insulator but underestimates the band gap. The recently-implemented screened hybrid functionals method (HSE06) represents only a moderate increase in computational effort compared to traditional DFT. This method allows one to modify the PBE-approximated exchange potential with a portion of the Hartree-Fock exchange. We present LDA, LDA+U, and HSE06 calculations of the density of states and band structure of NFO. We show that hybrid methods greatly improve agreement with the experimental band gap over LDA +U. We find that NFO is an indirect band gap system with the spin-down channel having the lower, indirect gap, whereas the majority channel possess a direct gap with over a 0.5eV difference with the minority gap. Comparison of our theoretical results with recent optical measurements on NFO thin films is also presented.

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