C10

Electronic structure of ferrimagnetic $NiFe_2O_4$ using the screened hybrid functional method

H. Sims, D. Mazumdar, W. H. Butler, and Arunava Gupta
Center for Materials for Information Technology (MINT)
Department of Physics
University of Alabama
Tuscaloosa, AL, U.S.A.
Q. Sun and J. Musfeldt
University of Tennessee
Knoxville, TN, U.S.A.

As an insulating ferrimagnet with a high Curie temperature, NiFe2O4 (NFO) may be a promising candidate for future spin-based applications. Recent demonstration of spin-Seeback effect in magnetic insulators proves that such materials are only beginning to be explored [1]. Unfortunately, density functional theory cannot give a full account of its properties; most notably, LDA and GGA calculations underestimate the band gap by several eV. Attempting to account for correlation effects through the addition of a Hubbard U does not yield a better answer. It is therefore necessary to utilize methods beyond standard DFT to accurately calculate the properties of this material. Although most computational methods that consider many-body effects prove (at times prohibitively) computationally expensive, the recently-implemented screened hybrid functionals method[2] represents only a moderate increase in computational effort compared to traditional DFT[3]. This method allows one to modify the local-density- or generalized-gradient-approximated exchange-correlation potential with a portion of the Hartree-Fock exchange. Although the method introduces some computational parameters, these parameters do not need to be fine-tuned to suit a given material in order to arrive at reasonable results. We present LDA+U, and screened hybrid functional calculations (HSE) of the density of states of NFO and an HSE calculation of the band structure and dielectric matrix.. 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. This is in agreement with recent optical experiments on high quality NFO thin films. Comparison of our theoretical results with experimental dielectric properties is also presented.

References

1) K. Uchida et. al Nature Materials **9** 894 2010

2) J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. **118**, 8207 (2003).

Jochen Heyd, Juan E. Peralta, Gustavo E. Scuseria, and Richard L. Martin. J. Chem. Phys. **123**, 174101 (2005).