First-principles study on magnetism and magneto-optical properties of yttrium iron garnet

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Yttrium iron garnet (YIG) is one of the key materials for applications to spintronic devices due to its characteristic low magnetic damping. Magnetism and magneto optical properties of YIG, with a chemical formula of $Y_3Fe_5O_{12}$, have already been widely investigated experimentally. Theoretical first-principles approach has also been applied to study the magnetism of YIG for the application of spintronic devices, however, there are difficulties to reproduce magnetism of YIG based on first-principles calculations due to the complexity of crystal structure and the strong interaction by the localized *d*-electron of the Fe atoms in YIG. Regarding the treatment of strong electron correlation, DFT+*U* method has become one of the most effective ways. This method can describe the electronic states by introducing the screened on-site Coulomb interaction in terms of Hubbard model parameter, U_{eff}. Previously, we have investigated the on-site Coulomb interaction in several simple transition metal oxides based on constrained DFT approach within a linear response theory [1]. We have additionally succeeded to describe the electronic structure of YIG and to obtain suitable U_{eff} value. In this work, we compute the magnetism of YIG by using the two values of U_{eff}, i.e. 9.8 eV for Fe atoms in octahedral 16(a) sites and 9.1 eV for those occupying the tetrahedral 24(d) sites. Calculations were carried out on the basis of the generalized gradient approximation [2] by using full-potential linearized augmented plane wave method [3]. We consider a bcc model of YIG (space group Ia-3d) which contains 160 atoms (80 atoms in the primitive cell), and the experimental lattice constant ($a = 12.376$ Å) [4] has been used in the calculations. Further discussion on magneto crystalline anisotropy and magneto-optical properties of YIG using the computed U_{eff} values will be presented.

[1] K. Nawa *et al*., Phys. Rev. B **97**, 035117 (2018).

[2] J. P. Perdew *et al*., Phys. Rev. Lett. **77**, 3865 (1996).

[3] K. Nakamura *et al*., Phys. Rev. B **67**, 14405 (2003).

[4] S. Geller *et al.*, J. Phys. Chem. Solids **3**, 30 (1957).