First principles calculations on electronic structure and magnetic properties of yttrium iron garnet

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Yttrium iron garnet (YIG) is one of the most studied magnetic insulators for application to spintronic devices. The electronic structure of YIG has been widely investigated experimentally. From the theoretical side, however, only few reports on the electronic structure are available due to the complexity of crystal structure and the strong interaction caused by localized *d*-electrons. Regarding the treatment of strong electron correlation, DFT+*U* method has become one of the most effective ways to deal with this problem. 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]. In the present work, this method is applied to describe the electronic structure of YIG. 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. Due to the presence of two inequivalent crystallographic positions of the Fe cations, we have obtained two values of U_{eff}, i.e. 9.6 eV for Fe atoms in octahedral 16(a) sites and 9.2 eV for those occupying the tetrahedral 24(d) sites. Further discussion on the electronic structure and magnetic properties of YIG using the computed U_{eff} values will be presented.

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