Machine-learning analysis of on-site Coulomb correction in yttrium iron garnet

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Yttrium iron garnet (YIG) is one of important insulating magnetic materials serving recent spintronic applications. However, due to a difficulty to treat the correlated electrons, the understanding of this material is still limited and thus the appropriate description of electronic structures is desirable. In first principles calculations based on density functional theory (DFT), the correlated electrons in localized *d* and *f*-electrons are practically treated by using the DFT+*U* method, which introduces the Hubbard-model parameters, on-site Coulomb (*U*) and the exchange (*J*) interactions, and is applied to complex systems containing a large number of atoms. The values of effective on-site Coulomb parameters, U_{eff}=*U*–*J*, are usually determined by fitting experimental results such as an energy band gap, optical spectra, and/or oxidation energy so as to obtain a good agreement with the calculated material properties. Thus, the choice of optimal U_{eff} values in a material is of crucial importance in an accurate description to electronic structure. In the present work, we have proposed new approach for seeking optimal U_{eff} values to simulate a complex dielectric function in experiments by using a combined neural network with first principles calculations, and applied this method to YIG with a garnet structure which contains 160 atoms and two inequivalent Fe cation sites surrounded by octahedral and tetrahedral oxygens in the crystallographic unit cell. First principles calculations were carried out based on the generalized gradient approximation by using the full-potential linearized augmented plane wave (FLAPW) method[1], where the U_{eff} values of Fe cations in the octahedral and tetrahedral sites, $U_{\mathrm{eff}}^{\mathrm{O}}$ and $U_{\mathrm{eff}}^{\mathrm{T}}$, were incorporated in the atomic limit approximation[2]. First, we calculated 35 data of dielectric functions for YIG by assigning various $U_{\mathrm{eff}}^{\mathrm{O}}$ and $U_{\mathrm{eff}}^{\mathrm{T}}$ values, ranging from 0 to 10 eV, each other by using FLAPW method, and constructed the neural network to learn a relationship between the dielectric functions and the U_{eff} values in YIG. Then, we sought the optimal U_{eff} values that fits experimental dielectric functions[3]. The result importantly predicted that the $U_{\mathrm{eff}}^{\mathrm{O}}$ and $U_{\mathrm{eff}}^{\mathrm{T}}$ behave differently, i.e., the values result in 5.34 eV for the $U_{\mathrm{eff}}^{\mathrm{O}}$ and 7.68 eV for the $U_{\mathrm{eff}}^{\mathrm{T}}$, due to the different valences. With these values, the calculated spectrum of the real part of the dielectric function shows the characteristic peak and shoulder at around 3-4 eV; the former is attributed in the electric dipole transition between 3*d* and 4*p* states in Fe at the tetrahedral site and the latter is that at the octahedral site. Detail discussion based on the band structure will be presented.

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