Effective on-site Coulomb interaction based on linear response theory for transition-metal monoxide thin films

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Density Functional Theory (DFT) has been commonly regarded as one of the most important tools to study the electronic structure of materials. However, DFT is insufficient to adequately describe the electronic structure of transition-metal oxides (MTOs) as it is impossible to fully treat the strong interaction caused by the localized electrons. As an alternative, DFT+*U* method has become one of effective means to deal with this problem. This method describes the electronic states by introducing the screened on-site Coulomb interaction in terms of Hubbard model parameter, U_{eff}. The U_{eff} values are commonly chosen to match experimental observations or calculated directly from first-principles calculations. However, various values for the U_{eff} have been reported even for the same ionic state and the same material. Since material properties are susceptible to the U_{eff} values, it is important to choose reliable ones. Previously, we have investigated the on-site Coulomb interaction in bulk 3*d* TMOs, based on constraint DFT approach within a linear response theory.[1] We here extend our approach to determine the U_{eff} values for thin films of 3*d* TMOs. Calculations were carried out based on the generalized gradient approximation[2] by using full-potential linearized augmented plane wave method.[3] With a model of a freestanding (001) monolayer, the in-plane lattice constants were fixed at experimental values of bulk TMOs and a ferromagnetic structure was assumed for simplicity. In the FeO monolayer, for example, the value of U_{eff} result is 1.74 eV when a unit cell including one TM atom is included. For a 4×4 supercell with sixteen TM atoms, it is converged to 9.13 eV. Furthermore, we confirmed the insulating characters obtained from DFT+*U* due to the localized 3*d* electrons. Details of the discussion, as well as those for other thin films of CoO and NiO, 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).