Ferromagnetism Induced by Vacancy Defect and Lattice Distortion in TiO_2 and ZnO

Dongyoo Kim, Jeonghwa Yang, Jisang Hong*
Department of Physics, Pukyong National University

Through the full potential linearized augmented plane wave (FLAPW) method, we have explored the vacancy defect induced magnetism in TiO_2 and ZnO . It has been found that the oxygen vacancy induces lattice distortion in rutile TiO_2, while there is no meaningful change in anatase structure. We have realized that the ferromagnetism in rutile TiO_2. stems from charge redistribution arising from the lattice distortion. The magnetic moment of 0.22 μB was found in Ti atoms neighboring oxygen vacancy site. Also, we have investigated the vacancy defect induced magnetism in wurtize ZnO. It has been found that the Zn vacancy defect brings a spin polarized state in the nearest neighbor oxygen atoms, whereas the oxygen vacancy defect has no influence on the magnetism. However, it is found that the lattice distortion is a crucial factor for the Zn vacancy induced ferromagnetism because the ferromagnetic ground state cannot be achieved if there is no lattice distortion due to Zn vacancy defect. The magnetic moment of oxygen atom in the nearest neighbor from the Zn vacancy site is ranged from 0.10 to 0.19 μB and the spin polarized oxygen atoms have metallic feature in both spin states. In addition, we have found that the ferromagnetic exchange interaction among oxygen atoms in mediated by Zn 3d state.

This work was supported by a Korea Science and Engineering Foundation (KOSEF) grant founded by the Korea government (MEST) (No. R01-2008-000-20014-0).