O-IV-3

The magnetic phase and the electronic structure of doped Gd-clustering for topological insulator, Bi_2Te_3

Eun-Ha Shin[1,*], Myung-Hwa Chung[2], Miyoung Kim[1], Hanchul Kim[1]
[1]Department of Physics, Sookmyung Women's University
[2]Department of Physics, Sogang University

The discovery of three dimensional strong topological insulators (TI) has intrigued many researchers. The surface metallicity in contrast to the insulating bulk state is known to be topologically protected by spin-orbit coupling and robust for impurities, disorders and the shape of material as long as the time reversal symmetry is preserved.

One of TI, Bi_2Te_3 was studied to examine whether topological surface state is hold when the magnetic transition metals such as Fe, Mn, and Co are doped. In this presentation, we report density functional theory calculations on the crystal of $Bi_{2-x}Gd_xTe_3$ (x=0.021, 0.042, 0.063, 0.074, 0.083, 0.125) to understand the effect of substitution of magnetic rare-earth element, Gd (Gd_{Bi}) on the surface metallicity and the magnetic property.

A single Gd_{Bi}'s in Bi_2Te_3 crystal (x=0.021) is calculated to carry a spin magnetic moment of 7 μ_B. Two Gd_{Bi}'s in Bi_2Te_3 crystal (x=0.042) prefer to be located in the first nearest neighbor sites in the Bi sublattice on a single Bi atomic layer of the same quintuple layer. The magnetic moments of two Gd_{Bi}'s remain unchanged (7 μ_B) and the antiferromagnetic (AFM) configuration is more stable [ΔE (=E_{AFM}-E_{FM}) is –2.36meV] due to super-exchange interaction via the intervening Te atoms.

With the increased concentration of Gd, we found that Gd_{Bi}'s favor to be clustered than to be uniformly dispersed. For instance, Gd_{Bi}'s form a linear chain (x=0.083) or a hexagonal ring (x=0.125) in the single Bi atomic layer. In most of the clustered structures, the AFM ordering is calculated to be more stable than the FM ordering. Among the considered configurations, the hexagonal ring is most effective in stabilizing the AFM phase (ΔE = -14.7 meV).