Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Impurities in Bi2Se3 topological insulator: ab initio calculation TOME M. SCHMIDT, ROBERTO H. MIWA, Universidade Federal de Uberlândia, ADALBERTO FAZZIO, Universidade de Sao Paulo — Topological insulators are materials that have a bulk as an ordinary insulator but have protected conducting states on their surface. The surface states with an odd number of Dirac cones are robust against time-reversal invariant perturbation. However the interaction of magnetic impurities with the Dirac fermions can break time reversal symmetry open unp a surface band gap. In this work we investigate the magnetic anisotropy and spin-texture of Co impurities embedded at the interlayer vdW spacings and onto the topmost Se network of the topological insulator Bi_2Se_3. The interaction of the magnetic impurity with the surface spin texture break time reversal symmetry, opening up a surface band gap. For Co atom adsorbed onto the surface, the net magnetic moment is aligned perpendicular to the surface plane, with anisotropy energy of 6$\sim$meV. On the other hand for the Co impurity at the vdW interlayers, the net magnetic moment is aligned in-plane. While pristine Bi_2Se_3 presents helical spin-texture in the massless surface Dirac cone and states resonant within the valence band, the presence of Co impurity reduces the planar spin helicity of now massive Dirac fermions. On the other hand O impurities do not break the protected surface Dirac cones, but they move the position of the Dirac crossing upwards. Also we observe that there is an energy barrier for the O_2 molecule when it approximates to the Bi_2Se_3 surface, but atomic O inside the Bi_2Se_3 is more stable than the formation of O_2 molecules.

Tome M. Schmidt
Universidade Federal de Uberlândia

Date submitted: 23 Nov 2011 Electronic form version 1.4