Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Metallic states in Topological Insulators with Magnetic Impurities[1] LEONARDO ABDALLA, ADALBERTO FAZZIO, Instituto de Física, Universidade de São Paulo, TOME SCHMIDT, ROBERTO MIWA, Instituto de Física, Universidade Federal de Uberlândia — Topological insulators are characterized by an insulating bulk, and an odd number of Dirac cones in the surface. Their existence are due a band inversion in the bulk phase created by a strong spin orbit coupling. Those metallic states have their spin polarization locked in a plane giving rise to a chiral spin texture, similar to the quantum spin hall effect. Such spin helicity suppresses backscattering processes. Based on first principles calculations, we performed a systematic study of transition metal (TM) impurities (Co, Mn, Ni, Cr and Fe) lying on the topmost layers of the Bi_2Se_3 topological insulator. Based upon formation energy results, by considering a number of plausible configurations, we find an energetic preference for the TMs occupying the topmost Bi substitutional site, and the subsurface interstitial sites neighboring Bi atoms. Our simulated scanning tunneling images (STM) show that there is local perturbation on the electronic structure of the surface. Further electronic band structure calculations indicate that (for some systems) the topologically protected surface metallic bands are suppressed, opening a band gap. In those systems the time reversal symmetry has been broken due to the formation net magnetic moment aligned perpendicularly to the surface plane.

[1]Work supported by CNPQ and FAPESP

Leonardo Abdalla
Instituto de Física, Universidade de São Paulo

Date submitted: 08 Nov 2012 Electronic form version 1.4