Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Large band gap quantum spin hall insulators of fluorinated Pb-X (X= C, Si, Ge, Sn) JOSE EDUARDO PADILHA, Universidade Federal do Parana - Jandaia do Sul, RENATO BORGES PONTES, Universidade Federal de Goias, TOME MAURO SCHMIDT, ROBERTO HIROKI MIWA, Universidade Federal de Uberlandia, ADALBERTO FAZZIO, Universidade de Sao Paulo — The Quantum Spin Hall Insulating (QSHI) phase was first observed in the HgTe/CdTe quantum well structure. However, the observed band gap of 5 meV is too small for practical applications. Other materials have also been proposed for the observation of the QSHI phase, such as silicene, germanene, stanene, and its halogenated phases. The spin-orbit interaction is a key feature in topological insulators, raising the interest in heavy elements, such as Bismuth. In fact, Bi is responsible for the high spin-orbit coupling that drives the band inversion in Bi_2Se_3 and Bi_2Te_3. Another element that also has a large spin-orbit interaction is Lead (Pb). Here we present a set of 2D QSH insulators with a very large band gap based on fluorinated Pb-X (X= C, Si, Ge, Sn). First-principles phonon dispersion calculations indicate that these systems are structurally and mechanically stable. By performing DFT-based electronic structure calculations we show that 2D Pb-X functionalized with fluorine are topological insulators with very large band gaps (over 0.7 eV). Addtional calculations, for nanoribbons structures, show the presence of a Dirac cone at the center of the Brillouin zone. These results can establish a new route to the observation of QSHI phase at room temperature.

Jose Eduardo Padilha
Universidade Federal do Parana - Jandaia do Sul

Date submitted: 04 Nov 2015 Electronic form version 1.4