Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Electronic Structure calculations in a 2D SixGe1-x alloy under an applied electric field[1] JOSÉ EDUARDO PADILHA, University of São Paulo, RENATO B. PONTES, Federal University of Goiás, LEANDRO SEIXAS, ANTÔNIO J.R. DA SILVA, ADALBERTO FAZZIO, University of São Paulo — The recent advances and promises in nanoscience and nanotechnology have been focused on hexagonal materials, mainly on carbon-based nanostructures. Recently, new candidates have been raised, where the greatest efforts are devoted to a new hexagonal and buckled material made of silicon, named Silicene. This new material presents an energy gap due to spin-orbit interaction of approximately 1.5 meV, where the measurement of quantum spin Hall effect(QSHE) can be made experimentally. Some investigations also show that the QSHE in 2D low-buckled hexagonal structures of germanium is present. Since the similarities, and at the same time the differences, between Si and Ge, over the years, have motivated a lot of investigations in these materials. In this work we performed systematic investigations on the electronic structure and band topology in both ordered and disordered SixGe1-x alloys monolayer with 2D honeycomb geometry by first-principles calculations. We show that an applied electric field can tune the gap size for both alloys. However, as a function of electric field, the disordered alloy presents a W-shaped behavior, similarly to the pure Si or Ge, whereas for the ordered alloy a V-shaped behavior is observed.

[1]This work is supported by CAPES, CNPq and FAPESP.

Jose Eduardo Padilha
University of São Paulo

Date submitted: 09 Jan 2013 Electronic form version 1.4