Abstract Submitted for the MAR07 Meeting of The American Physical Society

**Boron doped graphene nanoribbons** THIAGO MARTINS, Instituto de Fisica - Universidade de Sao Paulo, HIROKI MIWA, Instituto de Fisica, Universidade Federal de Uberlandia, ANTONIO J.R. DA SILVA, A. FAZZIO, Instituto de Fisica - Universidade de Sao Paulo — We will present a detailed study of the electronic, magnetic and transport properties of boron doped graphene nanoribbons, for various widths. The electronic structures and the equilibrium geometries were obtained through ab initio total energy DFT calculations. The transport properties were investigated using nonequilibrium Green's functions. Our results reveal that the substitutional boron atoms occupy the edge sites of nanoribbons, quenching the local ferromagnetism along the nanorribon edges. In addition, the presence of edge boron atoms break the symmetry between spin up and spin down transmittance channels. Those results suggest that, through a suitable doping process, it is possible to tailor the electronic current along the graphene nanoribbon. We thank FAPESP, CNPq and CENAPAD-SP.

> Thiago Martins Instituto de Fisica - Universidade de Sao Paulo

Date submitted: 15 Dec 2006

Electronic form version 1.4