Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic structure and magnetism in partially gated graphene nano-ribbons RITA MAJI, JOYDEEP BHATTACHARJEE, NATIONAL INSTITUTE OF SCIENCE EDUCATIONAND RESEARCH, BHUBANESWAR, ODISHA, INDIA — Properties of 3-coordinated carbon networks evolve upon physical or chemical functionalization depending on the resultant modification to π-conjugation and its interplay with the anti-ferromagnetic(AFM) correlation between unpaired $2p_z$ electrons at nearest neighbor(nn) sites. Although the former generally dominates the latter in determining the ground state, we propose it to be possible to enhance and modify nn magnetic correlations by inducing non-uniform density of electrons through application of bias partially within a periodic unit. Using tight-binding based mean-field Hubbard model and the DFT based first principles calculations, we show in ZGNRs as well as AGNRs, a systematic emergence of nn ferromagnetic(FM) correlation and spin-separation within and in the vicinity of positively biased region in a unit-cell, as an intermediate phase, as the ground state evolves from AFM to non-magnetic as a function of bias voltage. The associated evolution of the degenerate band-structure from direct to indirect is also punctuated by lifting of degeneracy coinciding exactly with the appearance of nn FM correlation and accommodating energy windows for half-metallic transport. In ZGNR such localization driven nn FM correlation leads to non-trivial edge magnetism and band-structure.

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Date submitted: 31 Oct 2015 Electronic form version 1.4