Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Novel quasi-1D Y-junction carbon with anisotropic conductance and changeable magnetization BHALCHANDRA PUJARI, Centre for Modeling and Simulation, Savitribai Phule Pune University, Pune 411007 India, ANDREY TOKAREV, DST Hydrogen Infrastructure Center of Competence (HySA Infrastructure), Faculty of Engineering, North-West University, Potchefstroom, South Africa
— We propose two conformations of a novel quasi-1D carbon allotrope designed by tailoring three graphene nanoribbons to form a Y-shaped junction. The armchair and zigzag conformations arise due to chirality of underlying ribbons. While armchair Y-junction carbon (YjC) is formed by three identical "arms" of the graphene nanoribbons the zigzag conformation has one distinguishable arm. The result in the later configuration is the broken symmetry of the structure, in which the arms are no longer separated by 120° each. Interestingly the broken structural symmetry of zigzag YjC is also associated with magnetic moment. It is shown that the magnetism is due to underlying nanoribbons and not symmetry breaking. Moreover the magnetism is also affected by the nature of edge passivation. Based on the analysis of density of states, we conjecture that the mixture of sp^3- and sp^2 bonded atoms results three conducting ribbons joined together by the insulating carbon chain. Thus making the structure an anisotropic conductor, with conductivity of armchair conformation being higher than that of zigzag. Armchair and zigzag conformations are energetically extremely stable with binding energy of 11.44 eV/atom and 8.39 eV/atom respectively.

Bhalchandra Pujari
Centre for Modeling and Simulation,
Savitribai Phule Pune University, Pune 411007 India

Date submitted: 07 Nov 2014 Electronic form version 1.4