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Title: Electron Transfer on Impurity doped Graphene Nanoribbon

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Graphene nanoribbons have bandgaps though the conductance and the valence bands touch at the K-point in graphene sheets. Using the graphene nanoribbons as the molecular devices, it has made possible to control the bandgaps. Since affinity of graphenes which are π-electron system is good for organic molecules, interesting physical properties are expected to apply for new devices by doping various atoms and molecules. By the computer simulation, we have numerically studied the electronic properties on the graphene nanoribbon with armchair shaped edges (AGNR) and zigzag shaped edges (ZGNR) doped various radicals. In this study, we have calculated the electronic structure by the first principle pseudo potential method based on the density functional theory (DFT) using the generalized gradient approximation (GGA). On our calculation, we have taken following conditions; the number of carbons of AGNR is 176, the k-point sampling is 256 points, the energy cutoff is 350 Rydbergs, and the bond length between carbons is 1.42 angstroms. We have optimized structures by the conjugate gradient (CG) method, then the bond length has been used for the initial distribution of carbon atoms and the size of the supercell. We have also calculated the electron transport in the nonequilibrium situation which considered connecting to the electrodes. We showed band structures of AGNRs doped various impurities. The impurity levels appear in the bandgaps of AGNRs when some molecules, CH_3, NH_2, OH are doped. On the other hand, no impurity levels of metals appear in the bandgaps. Properties of electron transports are calculated using the nonequilibrium Green?s function formalism through graphene nanoribbons. The transmission function is quantized against energies in non-doped AGNR, but the quantization becomes blunt in doped AGNRs. I-V characteristics of AGNRs are also evaluated from transmission functions. We have found that doped AGNRs have higher conductance than non-doped AGNRs