

Modeling Electrical Properties of Hetero-Junction-Graphene/Pentacene and Gold/Pentacene

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Abstract : We investigate the electronic transport properties across the graphene/ pentacene and gold/pentacene interface. Further, we studied the effect of ripples/bends in pentacene using NEGF-DFT approach. Current transport across the pentacene/graphene interface is found to be remarkably different from transport across pentacene/Gold interfaces. We found that current across these interfaces could be accurately modeled by a combination of thermionic and Poole-Frenkel emission. Further, the degree of bend or degrees of the curve formed during ripple formation strongly change the optimized geometric structures, charge distributions, energy bands, and DOS. The misorientation and hybridization of carbon orbitals are associated with a variation in bond lengths and carrier densities, and are the causes of the dramatic changes in the electronic structure during ripple formation. The electrical conductivity decreases with increase in curvature during ripple formation or due to bending of pentacene molecule and a decrease in conductivity is directly proportional to the increase in curvature angle and given by quadratic relation.

Keywords : hetero-junction, grapheme, NEGF-DFT, pentacene, gold/pentacene

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