Workfunction Tuning of Graphene with Organic Molecules

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Abstract

Graphene has conquered the field of Cutting Edge Technology as the ultimate next generation material. However, in order to be used widely in applications, one should be able to tune its electronic properties (i.e. *work function*). This may be achieved by deposition of electron acceptor or donor molecules on the surface of Graphene. In this work, we investigate the interaction between Graphene and an organic molecule, hexaazatriphenyl hexacarbonitrile (HATCN). HATCN is a strongly electron deficient molecule widely used in organic LEDs for hole injection [1,2]. By means of first principle computational techniques, we study the evolution in the work function of Graphene due to the adsorption of HATCN, as a function of the relative orientation and density of the doping molecules. Our modeling work points to a change from a lying-down to a standing-up configuration as the coverage increases, which is also observed in HATCN layer growth experiment over gold(111) and silver(111) surfaces [3,4]. The preferential standing-up configuration is confirmed by simulated Near Edge X-ray Absorption Fine Structure Spectra (NEXAFS) in excellent agreement with experimental data.

References

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