DESIGNING ALL-GRAPHENE NANO-JUNCTION BY EDGE FUNCTIONALIZATION: OPTICS AND ELECTRONICS

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The recent advances in production techniques of graphene nanostructures call for strategies towards all-graphene nanodevices. We study the effect of covalent edge functionalization on the opto-electronic properties of realistic graphene nano-flakes and junctions. By means of well tested semi-empirical methods, we compute both mean-field ground state electronic properties and configuration-interaction optical excitations. Our study shows that functionalization can be designed to tune electron affinities and ionization potentials of graphene nano-flakes [1]. This effect can be exploited to realize both type-I (straddling) and type-II (staggered) all-graphene nano-junctions. At variance to type-I [2], we find that type-II junctions can display indirect excitations with electrons and holes localized on different sides. The optical properties are characterized in terms of size and functionalization, and the conditions to obtain charge transfer excitons are discussed [3].

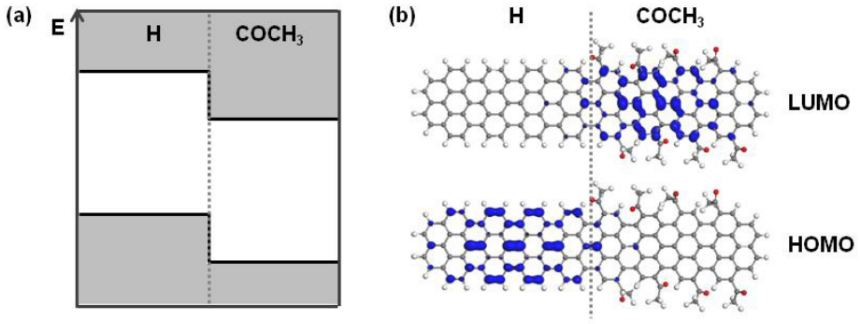

Figure 1: (a) Scheme for type-II graphene nano-junction: edge covalent functionalization with electron-withdrawing $COCH_3$ groups down shifts the gap region with respect to the hydrogenated side (H); (b) Localized frontier orbitals of H//$COCH_3$ nano-junction.

References

[1] C. Cocchi et al. J. Phys. Chem C dx.doi.org/10.1021/jp109909s (2011)
[2] D. Prezzi et al. Phys. Rev. B 77 (2008) 041404(R); D. Prezzi et al. to be published (2011)
[3] C. Cocchi et al. submitted (2011)