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Designing all-graphene nano-junctions by covalent functionalization CATERINA COCCHI, ALICE RUINI, S3 CNR-Nano & University of Modena, IT, DEBORAH PREZZI, S3 CNR-Nano, IT, MARILIA J. CALDAS, University of Sao Paulo, BR, ELISA MOLINARI, S3 CNR-Nano & University of Modena, IT
— We study the effect of covalent edge functionalization, with organic functional groups, on the opto-electronic properties of graphene nano-flakes and nano-junctions. We work within the frame of Hartree-Fock-based semi-empirical methods [1,2]. Our study shows that functionalization can be designed to tune electron affinities and ionization potentials of graphene flakes. The stability of the proposed mechanism is analyzed with respect to the functional groups, the functionalization rate and the width of graphene nanostructures. We show that this effect can be exploited to realize type-II all-graphene nano-junctions. Different frontier orbital alignments can be engineered varying the functionalization, leading to specific optical properties: The conditions to obtain charge transfer excitations are investigated.

[1] Dewar, et al., J. Am. Chem. Soc. 107, 3902 (1985)
[2] Ridley and Zerner, Theoret. Chim. Acta 32, 111 (1973)

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