The electronic structure of F and H on graphene and their effect on graphene's transport properties

Gonzalo Usaj
Centro Atómico Bariloche and Instituto Balseiro, CNEA, 8400 Bariloche,
and CONICET, Argentina

Using density-functional-theory, Hartree-Fock, exact-diagonalization, and numerical-renormalization group methods, we study the electronic structure of diluted F [1] and H [2] atoms chemisorbed on graphene. A comparison between DFT and Hartree-Fock calculations allows us to identify the main characteristics of the electronic structure of the defect. We use this information to formulate an Anderson-Hubbard model that captures the main physical ingredients of the system while still allowing a rigorous treatment of the electronic correlations. In addition, we study the transport properties of graphene in the strongly localized regime (induced by F impurities) where transport is characterized by the Mott variable range hopping regime and discuss it on the light of recent magneto-transport experiments [3].

[1] J. Sofo et al, Physical Review 83, 081411(R) (2011)
[2] J. Sofo et al, Physical Review 85, 115405 (2012)
[3] X. Hong et al, Phys. Rev. B 83, 085410 (2011)