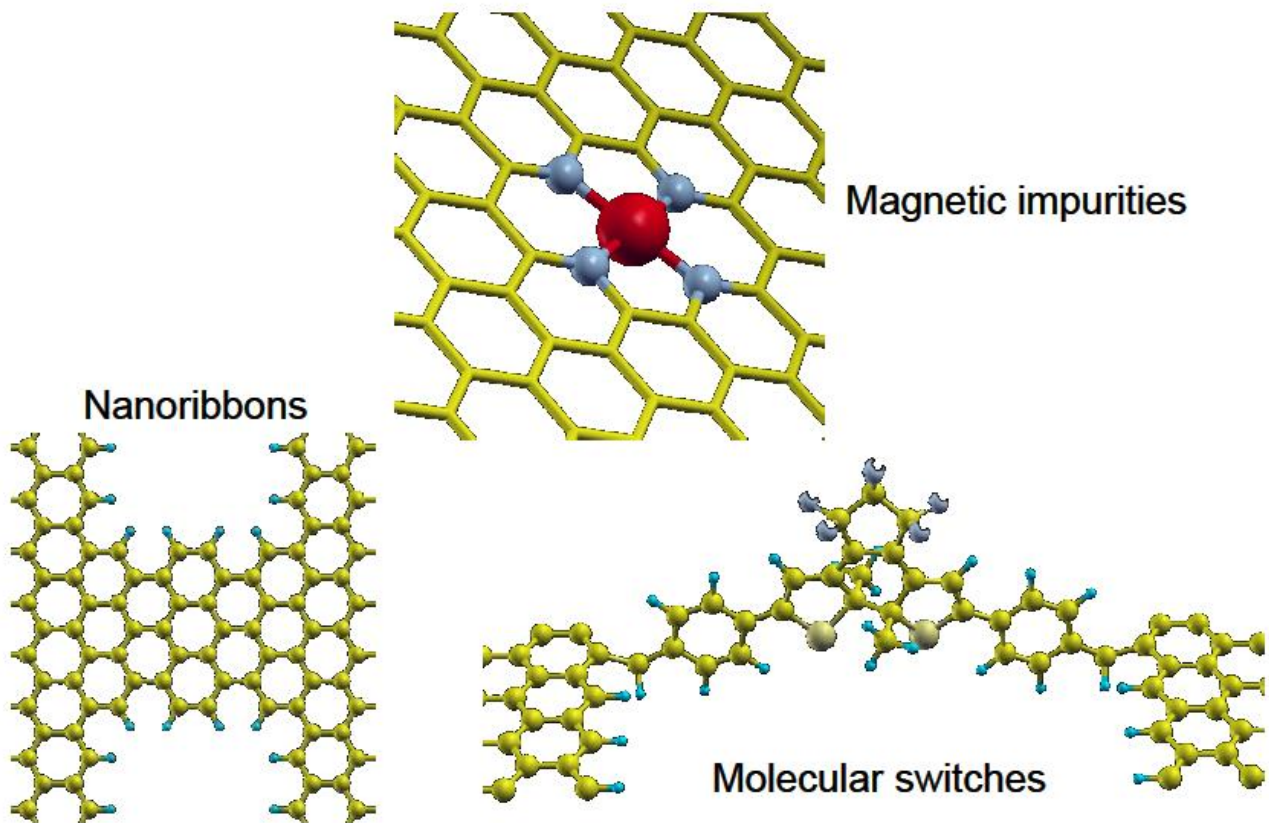


Modelling the electronic properties of functionalized graphene

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Graphene based materials are intensively studied being potentially useful in many different applications. In this talk after introducing the main graphene properties we plan to focus on two systems. Since magnetic effects can be induced through functionalization with magnetic impurities we shall deal firstly with graphene incorporating a FeN_4 molecule. In this case the transmission function with no applied bias shows a clear spin dependent behavior and consequently the electronic current exhibits a considerable spin polarization [1]. Second we shall treat a molecular switch constituted by a photochromic molecule with graphene electrodes. The conductivities are found to be very different for the two photochromic isomers. The almost zero density of states near the Fermi level of graphene enhances the effect of the HOMO and LUMO resonant states of the molecule in the conductivity which is less quenched with respect to a metal, e.g. Au and can be tuned by changing the end groups and the orientation of the molecule [2].



[1] S. Achilli et al: Spin dependent current and magnetic effects in FeN_4 -graphene, in preparation (2014).

[2] C. Motta, M.I. Trioni, G.P. Brivio and K.L. and K.L. Sebastian: Conductance of a photochromic-molecular switch with graphene leads, *Phys. Rev. B* 84, 113408 (1-5) (2011).