Spin asymmetric electronic structure of 3d transition metals on graphene

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Thanks to its unique properties, graphene is unanimously considered a very promising material to be used in various fields, such as energy production and storage, gas detection, and electronics. In particular, its application in spintronic devices is strictly related to the possibility of tailoring its magnetic properties, and extensive research in this field proved that adsorption of transition metal atoms fulfill this scope. In our study we considered the adsorption of the 3d transition metal atoms from Sc to Ni. The optimized geometries, electronic band structures and magnetic properties have been determined by means of periodic Density Functional calculations using the SIESTA and the CRYSTAL computational codes. The real space analysis of the electron density has been conducted within the formalism of the Quantum Theory of Atoms in Molecules (QTAIM) as impemented in the TOPOND code.
With the exception of Ni, the adsorbates induce large magnetic moments in the system. This spin asymmetry strongly affects the band structure of graphene, possibly opening spin asymmetric band gaps in the host material, as already observed in Fe@graphene.[1] Consistently, the QTAIM analysis reveals that the electron density transfer from the metal to the substrate, as well as the electronic rearrangement due to metal-carbon bonding, significantly depend on the spin component considered.

1. E del Castillo, F Cargnoni, S Achilli, G F Tantardini, M I Trioni, *Surface Science* **634** (2015) 62

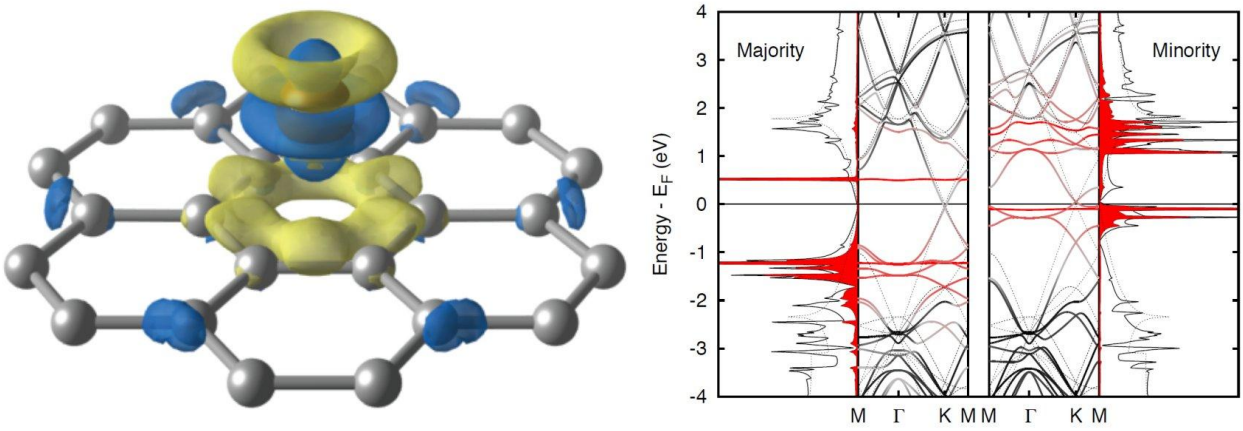

Figure 1. Electronic structure of Fe@graphene, 4x4 supercell. Left panel: deformation electron density. Right panel: density of states and band structure.