Influence of the spin-orbit interaction on the electronic properties of the graphene with the Ni-adatoms - a DFT study

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The electronic properties of the free standing graphene layer with Ni-adatoms is studied with the density functional theory approach, taking into account the spin-orbit interaction. We focus on the case when the Ni-adatoms form the trigonal lattice that is established above the graphene. The three geometries are examined, namely the Ni-adatoms in ontop, bridge and hollow positions on the graphene. We show that the presence of the metallic magnetic layer strongly modifies the band structure of the graphene, as well as its magnetic state. In the vicinity of the K-point the graphene valence band states are drag down below the Fermi energy, while the graphene conduction band states are less affected. We show that deformation of the Dirac cone results from the hybridization of the Ni *3d* and C $2p_z$ valence states. The presence of the magnetic adatoms generates the magnetic moments on the graphene lattice.

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