Doping induced Rashba spin splitting in graphene and planar BN

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Graphene and two-dimensional planar BN have emerged recently as very promising candidates not only for charge electronics but also for spintronics. Both pristine materials exhibit very long spin-lifetimes, owing to very tiny spin-orbit coupling in these materials. However, on the other hand, the very tiny spin-orbit interaction in these systems hinders many potential spintronic applications, where modulation of spin polarization is required. Therefore, as a remedy to this problem, the decoration of graphene layers with various atoms exhibiting stronger spin-orbit coupling has been proposed.

Here, we present non-perturbative fully relativistic *ab initio* calculations in the framework of density functional theory of the zero field spin splitting of energy bands in graphene and BN layers and nanoribbons functionalized by decorating pristine materials with Si, Ge, Sn, Pb, and Ca at various concentrations. In contrast to pristine graphene, the BN layers have considerable band gap, so it is interesting to figure out the role of the band gap on the doping induced spin splitting. As the first step, we calculate the equilibrium positions of decorating atoms on the graphene and BN planar backbones. Further, we calculate the relativistic band structure. Our calculations reveal the following scheme of electronic structure changes induced by decorating atoms in graphene. First, the decoration breaks the inversion symmetry of the pristine graphene, opens the band gap in K-point, and removes four-fold degeneracy in K-point. The spin-orbit coupling removes two-fold degeneracy and the linear-*k* spin splitting of Bychkov-Rashba type appears in the energy bands. From our *ab initio* calculations, we determine the magnitude of the constant in the Bychkov-Rashba effective Hamilltonian, and discuss the magnitude of this constant as a function of the adsorbate type and concentration. We consider also the functionalized graphene and BN nanoribbons, which allows us to determine the role of confinement on the magnitude of the zero field spin splitting and investigate magnetic moments at the edge states.

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