

Spin-orbit coupling caused spin splitting in doped graphene like layered materials

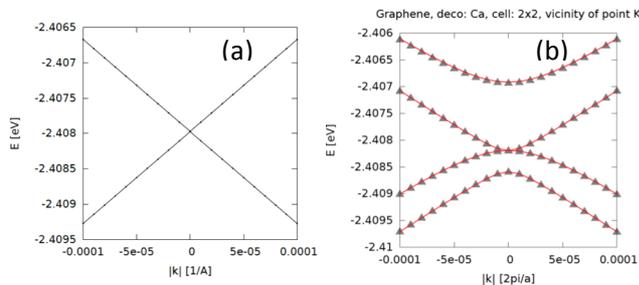
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We provide a general effective Hamiltonian, deduced from the theory of invariants, which describes relativistic band structure in pristine and decorated graphene-like systems for the most relevant region of low energy around the Dirac K -point. The effective Hamiltonian embraces systems such as decorated graphene (also silicene, germanene, and stanene), h-BN, and MX_2 (e.g., MoS_2). Together with relativistic *ab initio* calculations in the framework of the density functional theory (DFT) that provide the material constants, the developed scheme constitutes the general theory of spin splitting caused by the spin-orbit coupling (SOC) in layered materials. In this report, we provide exemplary results for graphene decorated with Ge, Sn, and Pb atoms (where the symmetry is lowered from the original D_{6h} symmetry to C_{3v}) and with Ca, and Sr (where the symmetry is lowered to C_{6v}).

Graphene and other two-dimensional systems have emerged recently as very promising candidates not only for charge electronics but also for spintronics. However, prerequisites for spintronic devices based on these systems are (i) deep quantitative understanding of the spin-orbit caused spin splitting in the electronic structure, and (ii) possibility to tune spin splitting by external factors, such as decoration of layers with various atoms.

The effective Hamiltonian for the band structure around the Dirac K -point (of the D_{3h} symmetry) has the form $H_{eff} = H_0 + H'$, where H_0 is usual low energy k.p Hamiltonian [1], and H' describes the effects of the perturbation (decoration) coupled to the S-O interaction, and was established by us on the basis of the theory of invariants [2]. It has the form of 4x4 matrix, $H' = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$, where $A = \begin{pmatrix} \Delta + \delta & 0 \\ 0 & \Delta - \delta \end{pmatrix}$ and $B = \begin{pmatrix} \Delta^* + \delta^* & 0 \\ 0 & \Delta^* - \delta^* \end{pmatrix}$, and contains four material constants, Δ , δ , Δ^* , δ^* , which can be determined from *ab initio* calculations. We perform DFT calculations taking relativistic effects non-perturbatively and employing relativistic PAW pseudopotentials as implemented in the *VASP* code. The full relaxation of atomic positions in the supercell is performed and provides us the energetically favorable position of the dopants in the graphene backbone. Extremely high degree of accuracy is enforced to be able resolve the electronic structure on the scale of μeV . For the case of Ca decorated graphene, the parameters of the effective Hamiltonian Δ , δ , Δ^* , and δ^* are computed to be equal [in eV] to -2.4076, 0.0006, -2.4084, 0.0002, respectively. The excellent agreement between the eigenvalues of the effective Hamiltonian and the electronic dispersions from DFT computations for the graphene decorated with Ca atoms (in the hollow position) at 13% concentration is illustrated in the figure below.



- (a) Dispersion relations for Ca decorated graphene (at hollow position) around the Dirac K -point (here taken as 0) with the spin-orbit coupling switched off. Here, the symmetry is high enough to cause crossing of doubly degenerated bands.
- (b) Spin splitting of bands around the K -point caused by S-O coupling obtained from the effective Hamiltonian (red lines) and DFT calculations (triangles).

We discuss also physical mechanisms leading to the constants in the effective Hamiltonian.

[1] See e.g., L. Brey and H. A. Fertig, *Phys. Rev. B* **73**, 235411 (2006).

[2] R. Winkler and U. Zülicke, *Phys. Rev. B* **82**, 245313 (2010).