

Spin-orbit coupling in dilute fluorinated graphene

Susanne Irmer, Tobias Frank, Denis Kochan, Martin Gmitra, Jaroslav Fabian

Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany
susanne.irmmer@physik.uni-regensburg.de

Abstract

Graphene and its various functionalized derivatives combine remarkable electronic and mechanical properties that make them feasible for novel electronic applications. From the point of view of spintronics it is crucial to understand spin-dependent phenomena that can be tuned and harvested from the newly engineered graphene-based materials. One of such materials is fluorinated graphene.

In the talk we present detailed *ab-initio* and tight-binding model studies focusing on spin-orbit coupling (SOC) effects in the fluorinated graphene. We discuss a new SOC mechanism which appears due to structural sp^3 distortion caused by chemisorption of fluorine and provide realistic values of induced SOC strengths.

The underlying tight-binding model is derived from symmetry considerations and its parameters are fixed by fitting to the *ab-initio* computed electronic band structure. The first-principles calculations were performed by means of full potential density functional theory (DFT) code [1]. We tested various supercell configurations, going from 5×5 supercell (fluorine-carbon ratio of 1 : 50) to 10×10 (fluorine-carbon ratio of 1 : 200). Our orbital and spin-orbital tight-binding models seem to be very robust. Their comparison with the first-principles results for the 10×10 supercell are shown in Fig. 1.

Figure 1(a) displays the orbital band structure and Fig. 1(b) the corresponding SOC splittings of valence, impurity and conduction band with respect to the Fermi level. These splittings are of the order of $100 \mu\text{eV}$. Based on the symmetry arguments we identify the main mechanism capable to explain SOC in the vicinity of fluorine. Moreover, testing our assumptions, we have turned off the SOC interaction on the fluorine atom in the DFT-calculation reaching typical graphene values, (order of $10 \mu\text{eV}$, see [2]), for more details consult Fig. 1(b). This reflects the fingerprint the SOC splitting of fluorine's atomic p orbitals leave in the SOC mechanisms and justifies our concentration on the impurity region.

The dominant contribution to SOC comes from the Bychkov-Rashba interaction and the new contribution which we called PIA SOC, see [3]. A similar Hamiltonian in the hydrogenated case was recently used in [3] to describe dilute hydrogenated graphene. We stress that the introduced SOC parameters are of the order of 10 meV and are thus remarkably larger than pristine graphene's intrinsic spin-orbit coupling of about 10^{-2} meV [2].

We conclude that the fluorine adatoms in small concentration induce a large SOC in graphene being about 1000 times larger than the intrinsic contribution of pristine graphene. This offers an inspiring initial point for further studies of SOC in dilute fluorinated graphene.

This work has been supported by the DFG SFB 689, GRK 1570, SPP1285, and the European Union Seventh Framework Programme under grant agreement 604391 Graphene Flagship.

References

- [1] FLEUR. <http://www.flapw.de/>
- [2] S. Konschuh, M. Gmitra and J. Fabian, Phys. Rev. B, **82** (2010) 245412.
- [3] M. Gmitra, D. Kochan and J. Fabian, Phys. Rev. Lett., **110** (2013) 246602.

Figures

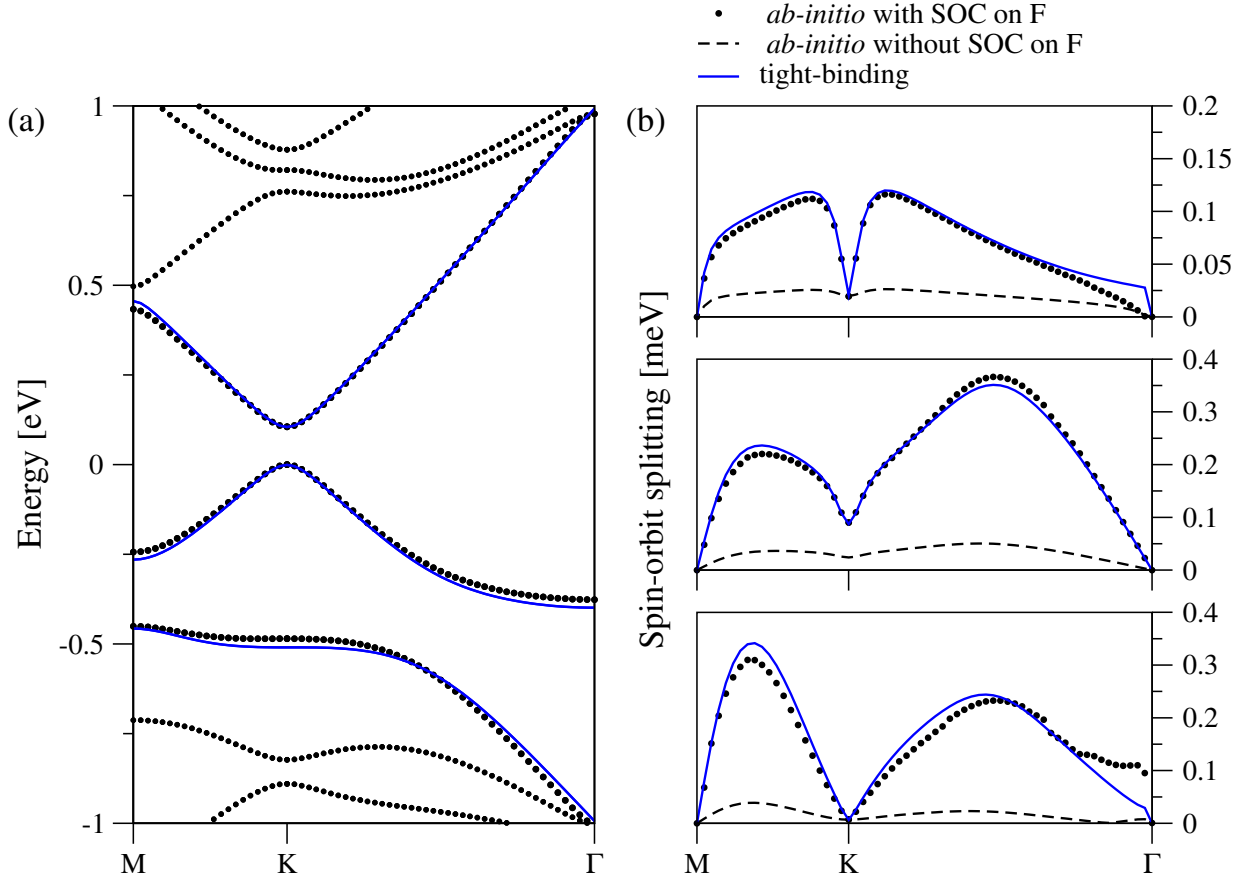


Figure 1: Band structure and spin-orbit coupling splitting of a 10×10 supercell calculation of fluorinated graphene. (a) Band structure around the Fermi level: The *ab-initio* data (black dotted lines) is fitted well by our tight-binding model (solid blue lines) around the Fermi level. (b) Band-splittings of corresponding valence, impurity and conduction band (bottom to top): Our tight-binding model (solid blue line) concentrating on the SOC in the vicinity of fluorine recovers the first-principles result (black dotted). Turning off the SOC on the fluorine adatom in the DFT calculation significantly reduces the splitting from about $100 \mu\text{eV}$ (dotted) to $10 \mu\text{eV}$ (dashed), which is of the order of the SOC induced splitting in pristine graphene.