# Electronic Structure of Stacking-Faults in Graphite

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The electronic structure of stacking faults (i) within hexagonal (AB) [1] and rhombohedral (ABC) [2] graphite, (ii) at the interface between both structures [3], and (iii) at a displaced surface layer on perfect crystals [1,2] has been investigated. A self-consistent, full-potential, density functional method (FPLO) has been applied. It turns out that all of the above mentioned interfaces induce strongly localized interface bands near the K-point in the Brillouin zone (BZ) (for an example see Fig.1), which give rise to strong peaks in the local density of states (LDOS) at the Fermi energy. Because the (L)DOS of the bulk materials at the Fermi energy is almost zero, the interface bands provide the dominating contribution to the local conductivity parallel and near the interface. We have also shown that the qualitative structure of the interface bands at the K-point in the BZ (i.e. their number and energy range) can be deduced from the geometrical structure of those atomic cluster at the perturbation, which are not present in the adjacent bulk structures, but produced by breaking the translational symmetry. These clusters are monomers, dimers, or linear trimers and linear tetramers depending on the geometrical structure of the interface. Only monomers and trimers produce interface bands at the Fermi energy. The other interface bands are located around $\pm 0.2$ eV (at tetramers), $\pm 0.4$ eV (at dimers), $\pm 0.5$ eV (at trimers), and $\pm 0.6$ eV (at tetramers). Observe, that the number of eigenstates of the model clusters and consequently also the number of interface bands due to a given cluster agrees with the number of atoms in the cluster. In the direction perpendicular to the layers, the interface bands at the K-point are almost completely localized within the clusters. Therefore, they form 2-dimensional electron systems which are weakly coupled to the adjacent bulk bands.

References

[1] M.Taut, K.Koepernik, and M.Richter, Phys. Rev. B **88**, 205411 (2013)
[2] M.Taut, K.Koepernik, and M.Richter, Phys. Rev. B **90**, 853121 (2014)
[3] M.Taut, K.Koepernik, and M.Richter, cond.mat. 1504.07812

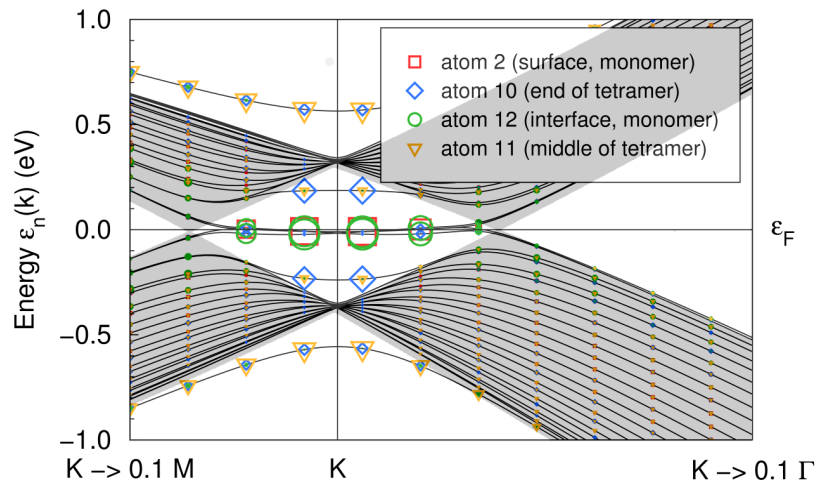Fig. 1. Band structure of the slab $(ABC)_4(BCA)_4$ in the vicinity of the K-point on the lines K-M and K-$\Gamma$. Orbital weights of $2p_z$-orbitals at some surface (No.2) - and interface (No.s 10-12) atoms are indicated by the size of the related symbols. Shaded areas denote the projected bulk band structure.