Symmetry of Electron Bands in Graphene: (Nearly) Free Electron Versus Tight-Binding

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Abstract We compare the classification of the electron bands in graphene, obtained by group theory algebra in the framework of a tight-binding model (TBM), with that calculated in a density-functional-theory (DFT) framework. Identification in the DFT band structure of all eight energy bands (four valence and four conduction bands) corresponding to the TBM-derived energy bands is performed and the corresponding analysis is presented. The four occupied (three σ-like and one π-like) and three unoccupied (two σ-like and one π-like) bands given by the DFT closely correspond to those predicted by the TBM, both by their symmetry and their dis-persion law.

However, the two lowest lying at the Γ-point unoccupied bands (one of them of a σ-like type and the other of a π-like one), are not of the TBM type. According to both their symmetry and the electron density these bands are plane waves orthogonal to the TBM valence bands; dispersion of these states can be determined unambiguously up to the Brillouin zone borders. On the other hand, the fourth unoccupied band given by the TBM can be identified among those given by the DFT band calculations; it is situated rather high with respect to energy. The interaction of this band with the free-electron states is so strong that it exists only in part of the k space.The symmetry labeling of all electron bands in graphene obtained by combining numerical band calculations and analytical analysis based on group theory is presented. The latter is performed both in the framework of the (nearly) free electron model, or in the framework of the tight-binding model. The predictions about relative positions of the bands which can be made on the basis of each of the models just using the group theory (and additional simple qualitative arguments, if necessary) are complimentary.

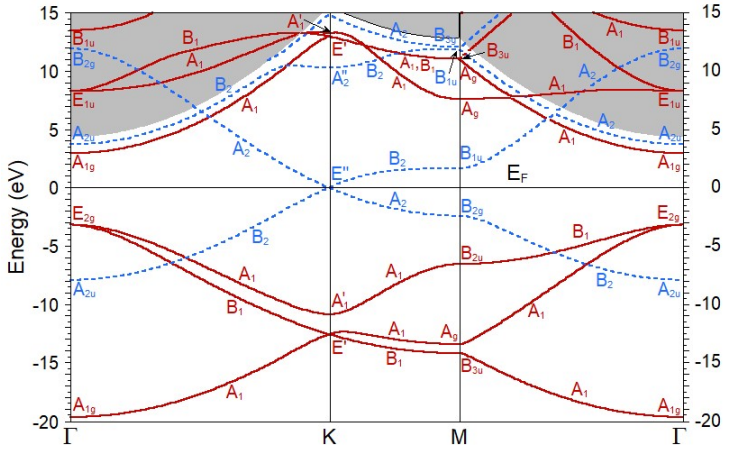

Figure 1: Calculated graphene band structure with labeling of states at the symmetry points and symmetry directions of the BZ. The σ-like bands are plotted with red solid lines and the π-like bands with blue dashed lines. The gray area corresponds to the vacuum continuum states. The black horizontal line shows the Fermi energy position

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