Evolution of p_z orbital with out-of-plane electric field in bilayer graphene

[1]JAIST, [2]Hitachi Cambridge Laboratory, ◦(D)K. Afsal,[1] M. Manoharan,[1] and H. Mizuta[1,2]
E-mail: afsal@jaist.ac.jp

An out-of-plane electric field has various effects on the physical properties of bilayer graphene (BLG) [1]. It is one of the methods used extensively to introduce the band gap in the BLG by breaking the symmetry between the top and bottom layers [2,3]. The immediate impact of the external electric field on the band structure of BLG reflects on the low energy bands such as valence band maximum (VBM) and conduction band minimum (CBM). Hence these two bands take a crucial role in the electronic properties of BLG. As is well known, the major contribution to the VBM and CBM comes from the out-of-plane p_z rbitals of individual C atoms. Thus herein, we study the evolution of the p_z orbital with the perpendicular electric field.

The *ab initio* calculations are performed using the LCAO method implemented in SIESTA [4] based on van der Waals exchange correlation functionals. A vacuum layer of thickness 20 Å was used to avoid the interaction between adjacent bilayers. A fine Monkhorst-Pack grid of 36 x 36 x 1 and a mesh cut off of 400 Ry were used in all the calculations. Wave functions are calculated using the utility Denchar, present in the SIESTA package.

Fig. 1(a) shows the band structure of bilayer graphene along the high symmetry points. The energy values are shifted so as to keep the Fermi level at 0 eV. Fig. 1(b) shows the wave function corresponding to the VBM (bottom line) and CBM (top line) at different perpendicular electric fields. As is evident from the figure, in the case of the VBM magnitude the p_z orbitals on the top layer of BLG shrink with the electric field and disappears at higher fields. As a consequence, the magnitude of the bottom orbitals increase. The CBM also shows the same behavior, but with a change in the role of the layers, as anticipated. This can be ascribed to the polarization of the orbitals in the presence of the electric field. Further details will be discussed in the presentation.

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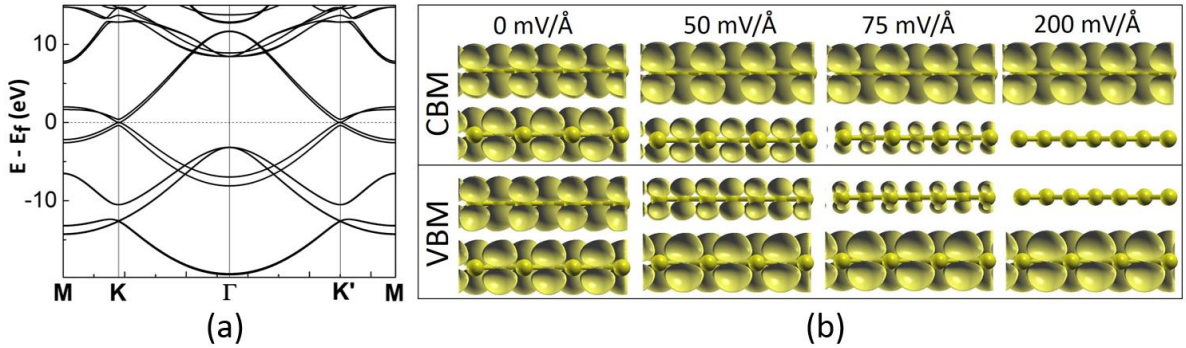

Figure 1: (a) Band structure of BLG along the high symmetry points. (b) Wave function corresponding to the VBM (bottom line) and CBM (top line) at different perpendicular electric fields (Isovalue: 0.15 $Å^{-3/2}$). In the case of VBM, magnitude of the p_z orbitals of the top layer shrinks and get accumulated at the bottom layer. The same effect is observed for the CBM, but with a reversal of the role of the layers.