Direct tight-binding calculations of band structure of asymmetrically doped twisted multilayer graphene

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Twisted bilayer graphene attracts the attention of surface science community lately due to prospects of isolated flat band formation at specific small twist angles (magic angles ~1^{o}) and, as a consequence, strongly correlated electron behavior, including possible superconducting state. Unfortunately, the unit cell of such twisted bilayer consists of thousands of atoms and calculation of band structure is a formidable task. Simplified continuum tight-binding (TB) models has been introduced, however in these models it is difficult to account various atomic relaxation phenomena as well as difference in doping levels generally appearing in real life. Also, the band structure generated for extremely large supercell is difficult to compare directly with experimental ARPES data which usually acquired for conventional graphene Brillouin zone (BZ), not the folded supercell BZ. Here, we report direct TB calculations using atomistic Slater-Koster approach for twisted multilayer graphenes with realistic asymmetric doping levels and also unfolded band structure in direct comparison with ARPES observations. The reduction of the Fermi velocity and formation of minigaps is obvious from calculations. Moreover adding more alternatively rotated layers reduces the band width more as shown in Fig. 1 (a).

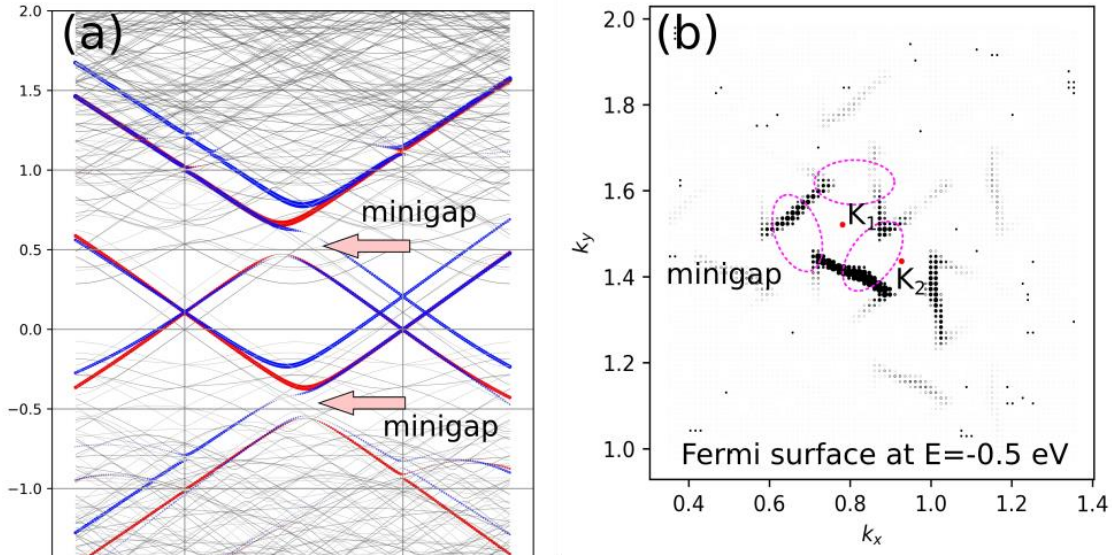

Fig. 1. (a) Comparison between band structure calculated for bi- (red) and trilayer (blue) unfolded bands of twisted multilayer graphene (θ~6^{o}). Light-grey are folded band manifolds. (b) Fermi surface at the energy corresponding to lower minigap in (a).