Theory and computation of the electronic band structures and optical absorption spectra for incommensurate twisted few-layers Graphene systems

Antoine Khater[1], Doried Ghader[1], Dominik Szczesniak[2]

[1] Université du Maine, IMMM UMR 6283, Avenue Olivier Messiaen, 72085 Le Mans, France
[2] QEERI-QF, Education City, Doha, Qatar

antoine.khater@univ-lemans.fr

Abstract

A theoretical method is presented to compute the electronic band structures and optical absorption spectra for the twisted *incommensurate* few-layers graphene (tLFG) systems of N arbitrary layers. This work integrates the recent and growing literature on the band structures of graphene systems as for example in [1-4], and on their optical absorption and scattering as in [5-7]. This method is developed using the virtual crystal approximation (VCA) and the tight-binding (TB) technique [8,9], where the VCA is achieved by a mathematical averaging formalism developed over the infinite ensemble of incommensurate interlayer structural configurations. The formalism goes beyond the Moire approximation [10]. Further, an important advantage of this approach is that it can be directly generalized for tFLG systems composed of any number N of graphene layers, whereas the Moire approach becomes impractical even for a twisted trilayer graphene. This approach is a first step in the development of a full CPA-TB theory taking into account the structural disorder of the N-tLFG systems.

Our computed results show that the low-energy electronic band structures of the incommensurate N-tLFG systems are formed of N overlapping Dirac cones centered on the K-points of the Brillouin zones of the graphene layers. Effective gaps between the saddle points of the valence and conduction bands of these systems are computed, and shown to be tunable with the incommensurate twist angles. The optical absorption spectra are also calculated for these systems in the same theoretical framework. In particular, the computed spectra display clear peaks which correspond to the accessible electronic transitions across the gaps between the valence and conduction bands of the incommensurate N-tLFG systems. The optical absorption results highlight the technical potential of these systems for applications in graphene based tandem cells. Figs.1 and 2 illustrate the computations for the N = 4 tFLG system.

References

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Figures

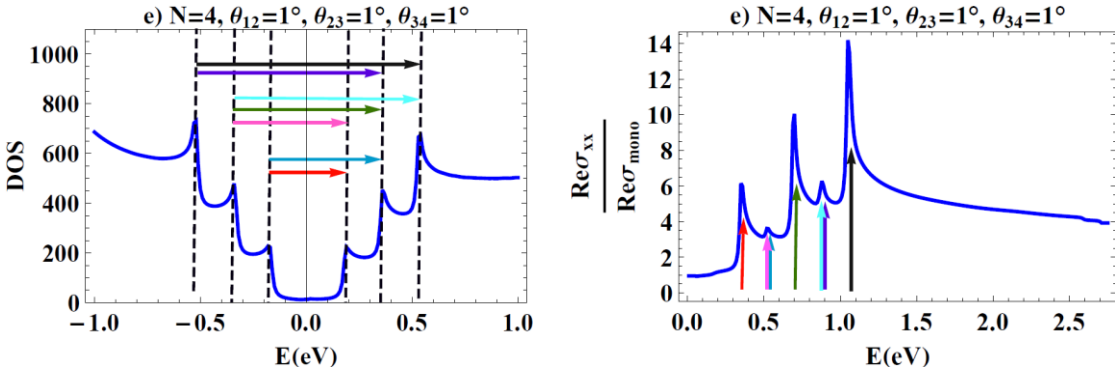

Fig.1: Calculated electronic DOS for the incommensurate tLFG graphene system of N = 4 graphene layers with one degree twist angles between adjacent layers.
Fig.2: Corresponding optical absorption spectrum, calculated at room temperature, and normalized with respect to the optical absorption spectrum for monolayer graphene.