TWISTED BILAYERS OF HEXAGONAL BORON NITRIDE

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Since the last decade, **twisted bilayers of graphene** (stackings of two graphene planes, with a non crystallographic rotation angle, also called *moires*) have attracted attention because novel -and quite fascinating- behaviours have been reported on these structures, especially when the angle of rotation is small [1]. Flat bands arise in electronic structure linked to different zones of the supercell, with local AA or AB stackings, and the resulting properties, such as Mott transition or tunable superconductivity, are controlled by a subtle interplay between the radius of these AA and AB stacking zones, the amplitude of interlayer interaction and the filling level.

More recently, the physical properties of **twisted bilayers of hexagonal boron nitride** (hBN) have been questioned. Differently to graphene, hBN is a wide band gap semiconductor (> 6 eV) and consequently attracts a growing interest for its strong UV photo-luminescence properties [2,3]. The optical properties of bulk as well as hBN layers are governed by strong excitonic effects. Theoretical studies of twisted hBN bilayer have been reported [Zhao, Wallet]. It has been shown for example that the rotation angle may be responsible for a geometric separation between the valence and conduction band states.

However, the geometries of stackings with a small angle of rotation require very large periodic cells, and the usual numerical approaches, mainly based on self consistent calculations, are restricted to a limited number of atoms in the calculation cell. In this context, and since we want to be able to calculate the electronic structure of twisted hBN bilayers with a wide range of rotation angles, only tight-binding (TB) approaches are tractable.

In the present work, we have extended a TB model originally developed for graphene moires [4] to the study of hBN twisted bilayers. First, the validation of this approach and its transferability to numerous systems will be discussed. More precisely, comparison with band structures of hBN bilayers calculated ab initio, for the smallest simulation cells will be presented including all the different stacking geometries which exist in such heteregenous BN system. In a second part, different electronic properties as well as optical properties will be investigated for various configurations, i.e. different angles and stackings.

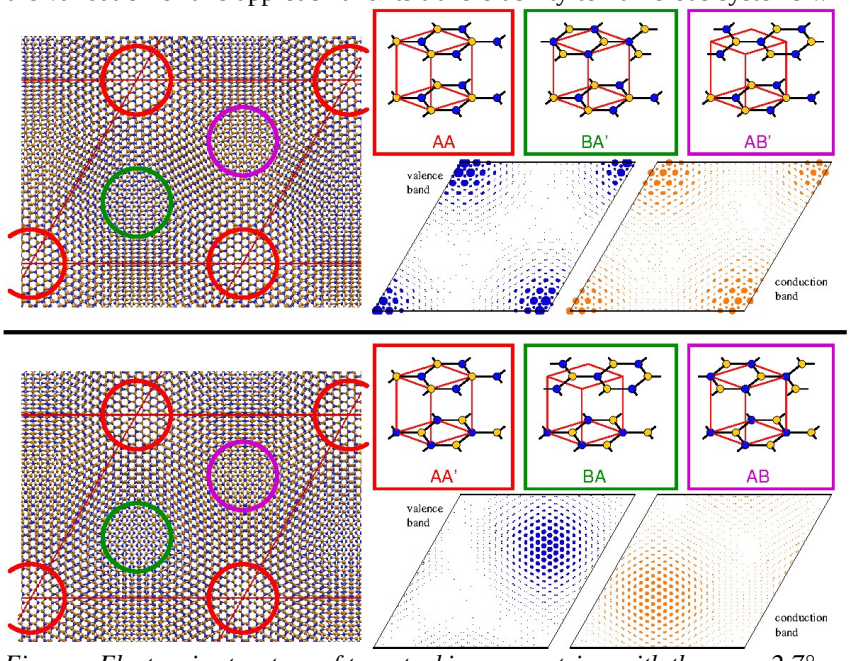

Figure : Electronic structure of two stacking geometries, with the same 2.7° angle (the only difference is a switch of B and N positions in the upper layer). Electronic states of both valence and conduction are localized in the high symmetry points areas. In the above case, valence and conduction belong to the same area. In the below case, eigenstates a geographically separated.

References

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