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Electronic localization in high-angle twisted boron nitride bilayer

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We investigate the electronic structure and the optical absorption onset of hexagonal boron nitride twisted bilayers at twist angles in the vicinity of 30° . Our investigations are done with ab initio density functional theories and a purposely designed tight-binding model. Despite its few parameters, we verify that the model ensures high precision on low-energy excitations. We demonstrate that approaching 30° , all stacking sequences tend to have the same band structure which is characterised by a bundle of flat bands laying slightly above the bottom conduction. The simulated independent-particle absorption spectra display an intense and well-defined peak at the onset, stemming solely from transitions to the bundle of flat states. These results suggest the presence of strong, stable and stacking-independent optical properties of boron nitride 30° -twisted bilayers. More importantly, the formation of flat bands and the indistinguishability of the stacking sequence, are expected to be common characteristics to all homobilayers made hexagonal monolayers at twist angles close to 30° . In fact, they are a consequence of the loss of translation symmetry (quasicrystal limit) occurring in all these systems at twists of exactly 30° .

The wide spectrum of physical properties exhibited by twisted bilayers has led to significant advances giving rise to the promising field of twistronics [1–5]. By stacking 2D atomic layers to form van der Waals heterostructures, a geometric moiré superlattice emerges as a result of a lattice mismatch or a rotational twist [6]. The resulting pattern modulates the potential at the supercell scale and hence changes the electronic band structure typically through the formation of low dispersing bands which possibly lead to peculiar transport characteristics, as unconventional superconductivity [7, 8] or insulating behavior driven by correlations [9]. Typical examples of moiré composites include the pioneering twisted bilayer graphene [10], twisted hexagonal boron nitride (hBN) [5, 11, 12], hetero- and homobilayers of transition metal dichalcogenides (TMDs) [13] as well as graphene on lattice-mismatched hBN substrates [14].

In this context, semiconducting twisted systems, like hBN or TMDs, are peculiar. In these bilayers, the width of band edge states decreases continuously with the angle of twist (no magic angle) and the presence of different atomic species generates several stacking possibilities with specific electronic properties, hence providing an additional degree of freedom with respect to graphene bilayers [15–17]. More specifically, hBN having the widest band gap in the monolayer (larger than 7 eV [18–21]) presents outstanding optical properties [22, 23] with many possible applications [24].

Since the early stages of the research on twist-angle physics, the scientific community has been investigating the small twist angle limit. In fact, there are no exhaustive theoretical studies in the literature about large-angle twisted bilayers. At best of our knowledge, only 30° twisted hBN bilayers [25] and graphene [26] have been considered. Even though density functional the-

ory (DFT) calculations suggest that this BN material is a new wide-gap 2D quasicrystal [25], its electronic and optical properties have never been addressed specifically. Very recently it has been highlighted in AlN and GaN binary materials [27] the emergence of localized states responsible of unique features. A similar physics is expected to occur also in large-angle twisted hBN bilayers. Most importantly, a 30° rotation produces quasicrystals without translational symmetry in all hexagonal bilayers, encompassing all most popular 2D materials like hBN, graphene, TMDs and their heterostructures, so all these systems must share some specific characteristics when twisted at large angles.

In this Letter, we determine the evolution of the band structure and optical response as a function of the twist angle in the vicinity of 30° for different stacking sequences of twisted hBN bilayers. By introducing a tight-binding (TB) model parametrized on DFT calculations, we show two surprising features. The first is that as the twist approaches 30° (the asymptotic quasicrystal limit), the electronic properties of all stackings tend to the same band structure. This can be understood by the fact that the system slowly approaches the asymptotic limit where it loses all translational symmetries. In other words, the system tends to a limit where all local configurations co-exist and the very notion of stacking sequence has no meaning. The second is that this common electronic

prefactor value (eV)	decay value	
γ^{BB}	2.45	q_{BB} 3.0
γ^{BN}	0.75	q_{BN} 2.0
γ^{NN}	0.32	q_{NN} 1.6

TABLE I. Set of parameters for the interlayer hopping.

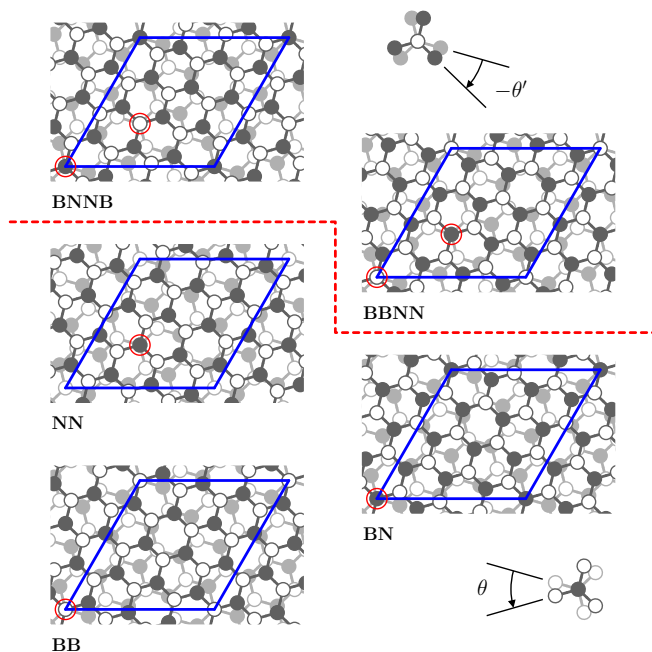


FIG. 1. The five hexagonal stackings of BN bilayers clasped into the single and double sublattice coincidence groups. Their stacking sequence takes the name from the atoms perfectly stacked at high symmetry points (red circles). The rotation angles are defined as the angles spanned by the B-N bonding at the coincidence point moving from the bottom layer to the upper layer.

structure is characterised by a strong electron localization resulting from the emergence of a bundle of low-dispersing states in the middle of the conduction band. We also show that, despite being in the middle of the conduction, the bundle is entirely responsible of a very intense and robust absorption onset which may give rise to spectacular excitonic properties.

To identify univoquely the structures we investigate, we use the definitions and nomenclatures that has been introduced in [17] by some of us. Let us recall the most important results for the current work. Every BN bilayer with hexagonal symmetry can be identified univoquely by a stacking label and a couple of integers (q, p) defining the moiré supercell. There are only five possible stacking sequences for each (q, p) -pair. The five stacking labels take their name from the pair of atoms placed exactly on top of each other on the three high-symmetry points of the hexagonal supercell that are the origin, the point $(1/3, 1/3)$ and the point $(2/3, 2/3)$. The five stackings divide into single-coincidence stackings (labelled BB, BN and NN) and double coincidence stackings (labelled BBNN and BNNB). The (q, p) indices define two matrices that, once applied to monolayer unitary vectors, generate the supercell of the lower layer and the twisted supercell of the top layer. If we take without loss of generality $p > q$, then the rotation of the top layer with

respect to the bottom layer is given either by an angle θ (in the single-coincidence systems) or $-\theta'$ (in the double-coincidence case) with $\theta' = \pi/3 - \theta$ (cfr. Figure 1. Both twist angles can be derived from p and q with formulae derived in [17].

In order to study in detail low-energy excitations in these systems, we developed a tight-binding model purposely designed to describe accurately the last occupied and the first empty states. We took inspiration from a previous model developed for graphene moiré bilayers [28, 29] and extended to twisted bilayer MoS₂ [30]. The basis is constituted of the p_z orbitals of B and N and the Hamiltonian relies on few parameters: the onsite energy difference $\Delta = 4.90$ eV between B and N species and the first-neighbour in-plane hopping $t_{\parallel} = -2.65$ eV. The interlayer hopping is included only for the σ components and has a distance-dependent form $t_{\perp}^{XY}(r) = \gamma^{XY} e^{-q_{XY}(a-r)/a}$ with a being the interlayer distance 3.22 Å [17], r being the distance between two sites belonging to different layers and XY labelling the pairings BN , BB and NN . The values of the γ^{XY} and q_{XY} parameters are reported in Table I. The quality of the model can be appreciated in Figure 2 where we report the top valence and bottom conduction states of the BB and the BN stackings at twist angle $\theta = 27.80^\circ$. These two stackings have been chosen as paradigmatic because of some specific characteristic of their band structure that

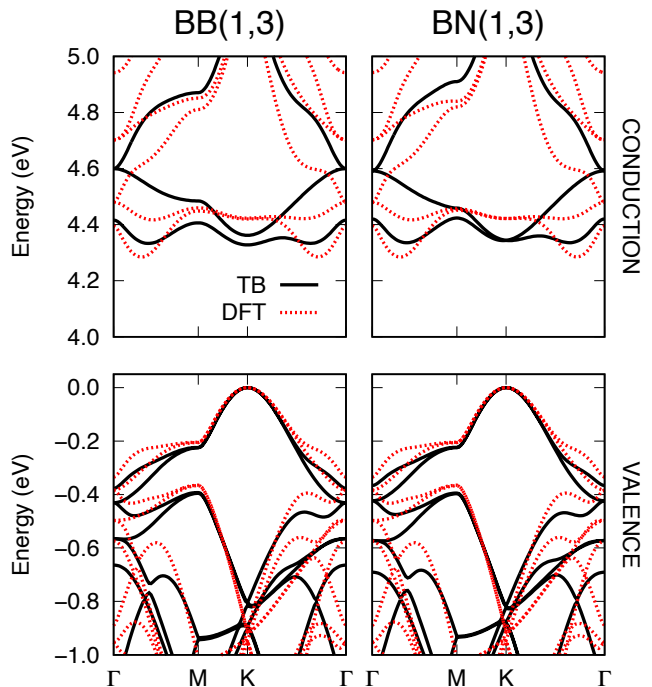


FIG. 2. DFT and TB bandstructure of the BB and BN stackings in the $(1,3)$ supercell, corresponding to a twist angle of $\theta = 21.79^\circ$.

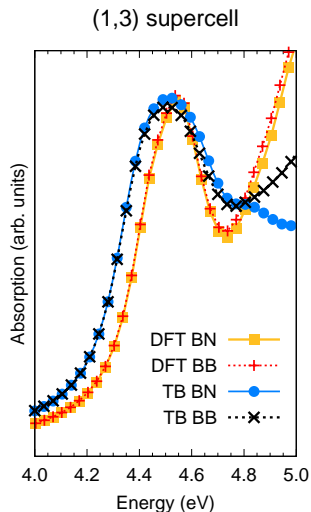


FIG. 3. Independent-particle absorption spectra of the BB(1,3) and BN(1,3) bilayers computed with *ab initio* and tight-binding methods.

is discussed in more detail below, and because the corresponding bilayers belong to two different layer symmetry groups. These have been computed with our TB model (black solid lines) and the DFT free simulation package Quantum ESPRESSO [31, 32] (red dashed lines).

Our TB model is parametrized to reproduce well some specific features of the band structure like the general dispersion of the electronic states and the gapwidth. Particular attention has been paid on the description of the two bands forming the bottom of the conduction. Indeed, the shape and the flatness of the bottom conduction bands are correctly reproduced by the model as well as the ordering. In fact, the DFT predicts the formation of a pretty flat dispersion in the M-K region in both systems. Actually the two bands avoid each other in the BB(1,3) electronic structure, even though the splitting is extremely small, whereas they cross at K in the BN(1,3), consistently with what simulated at smaller angles [17]. Our model catches very well these features although the splitting in the BB stacking is somewhat overestimated.

The imaginary part of the independent-particle transverse dielectric function $\varepsilon(\omega)$ at first order in the coupling with the vector potential $\mathbf{A}(\mathbf{r}, t)$ is obtained through the formula [33]:

$$\varepsilon(\omega) = \frac{e^2 \pi}{m_0^2 \varepsilon_0 \omega^2} \sum_{\mathbf{k}, m, \mu} |v_{\mathbf{k}\mu m}(\hat{\mathbf{e}})|^2 \delta(E_{\mathbf{k}\mu} - E_{\mathbf{k}m} - \hbar\omega), \quad (1)$$

where e is the absolute value of the electron charge, m_0 is the electron mass and ε_0 is the vacuum permittivity. This expression describes the absorption of a photon with energy $\hbar\omega$ and polarization vector $\hat{\mathbf{e}}$ through the promotion of an electron from the valence state $|m, \mathbf{k}\rangle$ of energy $E_{\mathbf{k}m}$ to the conduction state $|\mu, \mathbf{k}\rangle$ of energy $E_{\mathbf{k}\mu}$. The

velocity matrix element $v_{\mathbf{k}\mu m} = \langle \mu, \mathbf{k} | \hat{\mathbf{e}} \cdot \hat{\mathbf{v}} | m, \mathbf{k} \rangle$ is obtained from the eigenstates of the operator $\hbar\hat{\mathbf{v}} = i[\hat{\mathbf{H}}, \hat{\mathbf{r}}]$. We evaluated $\varepsilon(\omega)$ in the same systems as before using eigenvalues and eigenfunctions coming from our DFT calculations, by means of the Yambo [34] code, and from our TB model. Results are reported in Figure 3. Both methods predict a well-detached peak at 4.5 eV, corresponding to transitions towards the bottom conduction states. As expected from the electronic structure, differences between the two stackings are essentially negligible, indicating that not only the band structure but also the corresponding wavefunctions are remarkably similar.

Now that we have validated the TB model, we can extend our investigation to twist angles closer to 30° and systems that can hardly be addressed with DFT. In Figure 4 we report the bottom conduction states of the five stackings in the supercells (3,8), (4,11) and (11,30) corresponding to twist angles ranging from 29.41° to 29.96° in the single coincidence stackings (BB, BN and NN) and from 30.59° to 30.04° in the double coincidence ones (BBNN and BNNB). The tendency observed already in the (1,3) supercells is here confirmed and strengthened: all stackings present basically the same band structure at fixed supercell.

More interestingly, many low-dispersing states forming a bundle of flat bands are present above the bottom conduction and concentrated in an interval ΔE centered around 4.40 eV and pretty narrow (about 100 meV). Quite interestingly, this interval is at about the same energy where the M-K flat region was encountered in the (1,3) stackings (cfr. Figure 2). Such behaviour is in contrast to small-angles twisted hBN bilayers where one or more single states are formed directly in the gap and

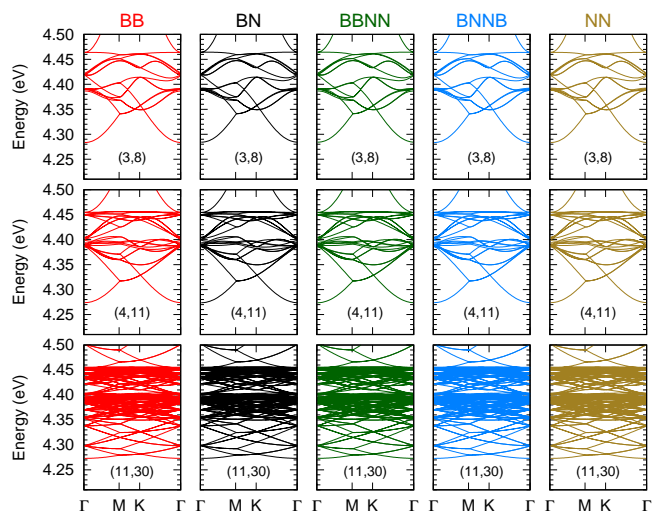


FIG. 4. From top to bottom: Bundle states in the conduction bands of the (3,8), the (4,11) and the (11,30) supercells of all the five stacking sequences (in different colors).

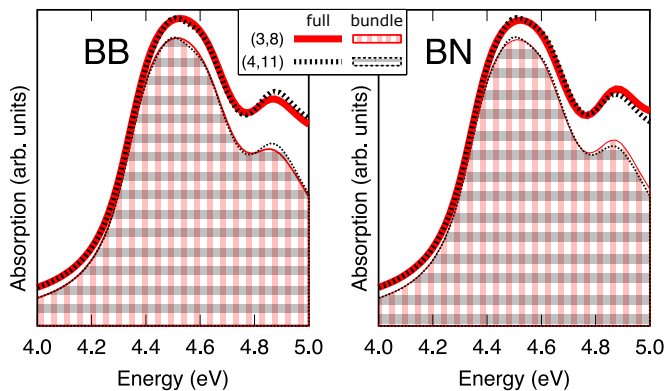


FIG. 5. Normalised independent-particle absorption spectra at the onset. BB stacking in the left panel, BN stacking in the right panel. Supercells (3,8) and (4,11) in black dashed and solid red respectively. Patterned areas stand for spectra obtained including allowing μ of equation (1) to run only on the bundle state index.

clearly separated in energy by about 0.1 eV [5, 11, 15]. Furthermore, BN being recognized as a cardinal compound in 2D material research for its exceptional optical features, it is therefore particularly worthwhile to understand the impact of these emerging states on absorption properties.

To this aim we computed with TB the independent-particle absorption spectra of the BB(3,8), the BB(4,11), the BN(3,8) and the BN(4,11) bilayers and we report them in Figure 5 as red solid and black dashed lines. As in the case of the (1,3) stackings, the spectral onset is dominated by a very intense and well detached peak at an energy compatible with the bundle states. As a confirmation of its origin, we computed the spectra including only transitions toward the bundle states (shaded patterns). We recover the same peak at essentially the same intensity indicating that, despite being in the middle of the conduction band, the bundle states are responsible of the absorption onset, the bottom conduction contributing only at higher energies.

To conclude, we have investigated the electronic and optical properties of hBN bilayers at twist angles close to 30° . To this aim, we have developed a simple and versatile tight-binding model which accurately describes low-energy excitations in all stacking sequences and twist angles. Its parametrisation has been validated against *ab initio* calculations of band structure and optical absorption. With our model, we have demonstrated that at twist angles close to 30° all hBN bilayers develop the same electronic properties, irrespective to the stacking sequence. This common electronic structure is characterised by the emergence of a bundle of low-dispersing states right above the bottom of the conduction band which are responsible of an intense and robust peak at the onset of the absorption spectrum. Our results suggest that 30° -twisted BN bilayers may host extremely

strong excitonic phenomena independent on the stacking sequence. More generally, the tendency of developing the same electronic structure is a consequence of the fact that any hBN bilayer becomes a quasicrystal in the 30° limit, i.e. a structure with no translation symmetry where all the possible local configurations co-exist. Since this very characteristic is actually common to the majority of homobilayers, we predict that a similar trend can be found in the 30° limit in all most common 2D materials including graphene, transition metal dichalcogenides, buckled graphene structures (antimonene, silicene), transition metal monochalcogenides, and all homostructures formed of hexagonal single-layers.

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