Emergence of flat bands in the quasicrystal limit of boron nitride twisted bilayers

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We investigate the electronic structure and the optical absorption onset of hexagonal boron nitride bilayers at small twist angles [1] and for twists in the vicinity of 30° [2]. Our study is carried out with a tight-binding model that we developed on purpose and validated against DFT simulations. We demonstrate that approaching 30° (quasicrystal limit), all bilayers sharing the same moiré supercell develop identical band structures, irrespective of their stacking sequence. This band structure features a bundle of flat bands laying slightly above the bottom conduction state which is responsible for an intense peak at the onset of independent-particle absorption spectra. These results reveal the presence of strong, stable and stacking-independent optical properties in boron nitride 30°-twisted bilayers. By carefully analyzing the electronic spatial distribution, we elucidate the origin of these states as due to interlayer B-B coupling. We take advantage of the the physical transparency of the tight-binding parameters to derive a simple triangular model based on the B sublattice that accurately describes the emergence of the bundle. Being our conclusions very general, we predict that a similar bundle should emerge in other close-to-30° bilayers, like transition metal dichalcogenides, shedding new light on the unique potential of 2D materials.

References

[1] S. Latil, H. Amara, and L. Sponza, SciPost Phys. 14, 053 (2023).
[2] L. Sponza, B. V. Vu, E. Serrano Richaud, H. Amara, and S. Latil, arXiv:2310.02937 (2023)

Figures

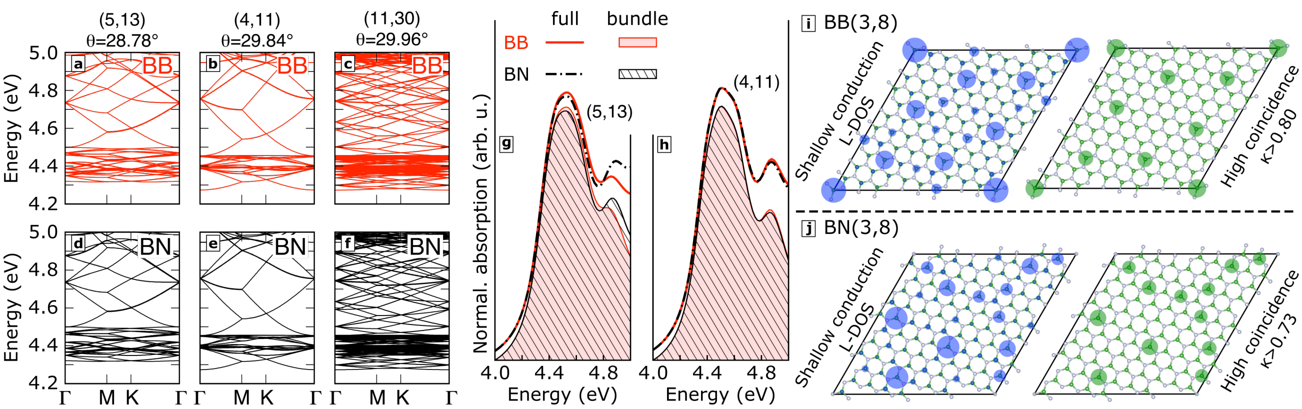

Figure 1: *(a-f)*: Conduction bands of different bilayer stackings at different twist angles close to 30°. *(g, h)*: Independent-particle absorption spectra including all empty states or only those in range 4.34 eV to 4.48 eV. *(i,j)*: Local DOS (blue cricles) and B-on-top-of-B map (green circles).