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 with twist angles in the vicinity of 30°. 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.