The twist angle dependence of quasi-Brillouin zones in doubly aligned graphene/BN heterostructures

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Controlling the relative rotation of two layers of two-dimensional materials has emerged as a compelling way to investigate the effects of a tunable periodic potential - the so-called moiré superlattice [1]. The periodic moiré potential can extend several orders of magnitude beyond the primitive unit cell and therefore reconstruct the electronic band structure of these materials, enabling exploration of novel correlated quantum phases [2-5]. In multilayer moiré heterostructures, interference between multiple twist angles typically produces tunable ultralong-wavelength patterns called supermoiré lattices, which can further reshape the host materials' electronic structure. These supermoiré lattices allow access to quasi- and nonperiodic regimes, resulting in a complex dependence on twist angles. In this talk, we discuss how the electronic properties of doubly aligned graphene/BN heterostructures evolve with angular alignment (see Fig.01) [6]. In addition to primary moiré and supermoiré effects, ill-defined periodicity - manifested as quasi-Brillouin zones - strongly affects the electronic structure, giving rise to new mini-gaps. Atomistic simulations clarify these features and highlight the important roles of lattice relaxation and quasi-commensurability of the primary moiré patterns.

References: **[1]** E.Y. Andrei and A.H. MacDonald, Nat. Mater. **19**, 1265–1275 (2020); [2] Y. Cao, et al., Nature **556**, 43-50 (2018); **[3]** G. Chen, et al., Nat. Phys. **15**, 237-241 (2019); **[4]** M. Serlin, et al., Science **367**, 900-903 (2020); **[5]** Z. Zheng, et al., Nature **588**, 71-76 (2020). **[6]** J. Vallejo Bustamante, et al., arXiv:2510.19369.

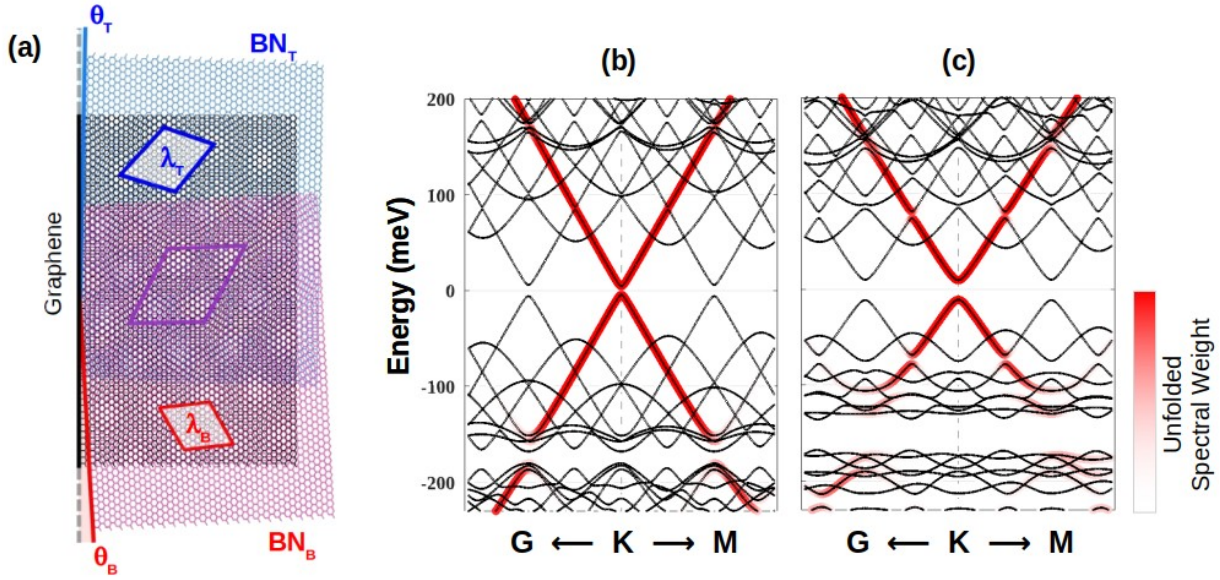

Fig.1: (a) hBN-encapsulated graphene heterostructure. (b,c) Electronic structure computed in two cases exhibiting the single moiré (θ_T=30°) and supermoiré (θ_T=-0.59°) effects, respectively, with θ_B=1.25°.