Flat bands and excitons in transition metal dichalcogenide moiré patterns

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Moiré patterns of 2D van der Waals materials have proven to be an ideal platform to host unusual correlated electronic phases, emerging magnetism, and exciton physics. At small twist-angles, novel moiré exciton states in transition metal dichalcogenide (TMD) heterostructures have been recently discovered through the observation of multiple emergent peaks in the optical spectra, but their atomistic nature has been a mystery. Using first-principles GW-Bethe Salpeter equation calculations we discover a rich diversity of excitonic states in large-area TMD moiré superlattices, particularly a novel exciton with an intralayer charge-transfer character [1]. We uncover a complex interplay between structural reconstruction, the formation of flat bands, and the nature of excitonic states [2]. These studies, which involve thousands of atoms in the reconstructed moiré unit-cell, are made feasible by the development of a new computational approach [1,3].

While small twist-angles have been widely studied, large twist angle superlattices are often considered electronically layer-decoupled due to misaligned Brillouin zones of the individual layers. Surprisingly, we observe the emergence of flat electronic bands with a distinctive anisotropic dispersion at a large magic twist angle in TMD bilayers (Fig. 1). A direct consequence of this flat band is the emergence of phonon-assisted intervalley absorption peaks in reflection contrast spectra measurements. The flat band shows a power-law divergent density of states due to its quasi-one-dimensional character, enhancing the potential for correlated phases.

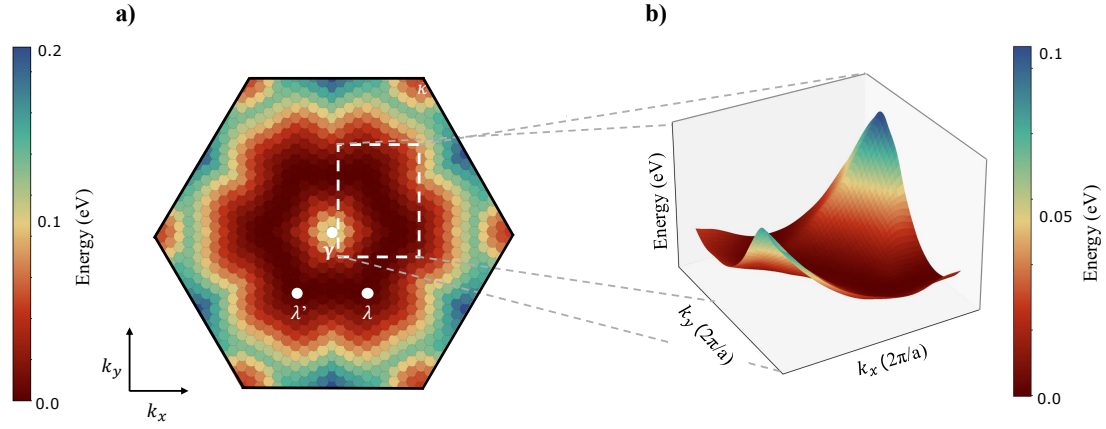

Figure 1 a) Distribution of the conduction band energy in the moiré Brillouin zone. b) cross-section of the flat band showing the quasi-1D character.

[1] MH Naik, EC Regan, Z Zhang, et al. Nature 609 (7925), 52-57 (2022)
[2] S Susarla, MH Naik, DD Blach, et al. Science 378 (6625), 1235-1239 (2022)
[3] H Li, S Li, MH Naik, et al. Nature materials 20 (7), 945-950 (2024)

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