Flattening conduction and valence bands for interlayer excitons in twisted van der Waals bilayers

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Recent advances in fabrication and manipulation of two-dimensional (2D) materials have enabled the control over stacking and twisting between layers of transition metal dichalcogenides (TMDs) in van der Waals (vdW) heterostructures. In these systems, the moiré pattern created by the lattice mismatch between the layers plays an important role: it produces a periodic potential profile along the plane for electrons and holes, with potential minima in regions with specific stacking orders. Such moiré superlattice potential leads to a band structure for the bilayer that is tunable e.g. by inter-layer twisting. The recent observation of Mott insulator and superconducting phases in twisted bilayer graphene [1,2], due to the band flattening induced by interlayer twist, has brought even further excitement into this field, towards controlling transport and opto-electronic properties of TMDs vdW heterostructures by similar moiré pattern effects. [3]

In this work, we explore the flatness of conduction and valence bands of interlayer excitons in MoS_2/WSe_2 van der Waals heterobilayers, tuned by interlayer twist angle, pressure, and external electric field. We employ an efficient continuum model [4] where the moiré pattern from lattice mismatch and/or twisting is represented by an equivalent mesoscopic periodic potential. We demonstrate that the mismatch moiré potential is too weak to produce significant flattening. Moreover, we draw attention to the fact that the quasi-particle effective masses around the Γ-point and the band flattening are *reduced* with twisting. As an alternative approach, we show (i) that reducing the interlayer distance by uniform vertical pressure can significantly increase the effective mass of the moiré hole, and (ii) that the moiré depth and its band flattening effects are strongly enhanced by accessible electric gating fields perpendicular to the heterobilayer, with resulting electron and hole effective masses increased by more than an order of magnitude leading to record-flat bands. These findings impose boundaries on the commonly generalized benefits of moiré twistronics, while also revealing alternate feasible routes to achieve truly flat electron and hole bands to carry us to strongly correlated excitonic phenomena on demand.

[1] Yuan Cao, Valla Fatemi, Ahmet Demir, Shiang Fang, Spencer L. Tomarken, Jason Y. Luo, Javier D. Sanchez-Yamagishi, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras, Ray C. Ashoori, and Pablo Jarillo-Herrero, Nature **556**, 80 (2018).

[2] Yuan Cao, Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras, and Pablo Jarillo-Herrero, Nature **556**, pages 43 (2018).

[3] Hongyi Yu, Gui-Bin Liu, Jianju Tang, Xiaodong Xu, and Wang Yao, Sci. Adv. **3**, e1701696 (2017).

[4] Sara Conti, Andrey Chaves, Tribhuwan Pandey, Lucian Covaci, François M. Peeters, David Neilson, Milorad V. Milošević, arXiv:2303.07755