Science Advances
AAAS

advances.sciencemag.org/cgi/content/full/6/42/eabc5638/DC1

Supplementary Materials for

Shedding light on moiré excitons: A first-principles perspective

Hongli Guo, Xu Zhang, Gang Lu*

*Corresponding author. Email: gang.lu@csun.edu

Published 16 October 2020, *Sci. Adv.* **6**, eabc5638 (2020)
DOI: 10.1126/sciadv.abc5638

This PDF file includes:

Table S1. **Twist angle dependent band width and exciton binding energy.** The variation of interlayer distance (δ*h*), VBM bandwidth, and exciton binding energy as a function of twist angle.

Angle (°)	3.5	6	9.56	21.7	32.2	0	56.5
δ*h* (Å)	0.54	0.44	0.22	0.02	0.02	0.00	0.58
VBM bandwidth (meV)	7	25	111	617	345	1500	3
Exciton binding energy (eV)	0.43	0.42	N/A	0.43	0.39	0.50	0.42

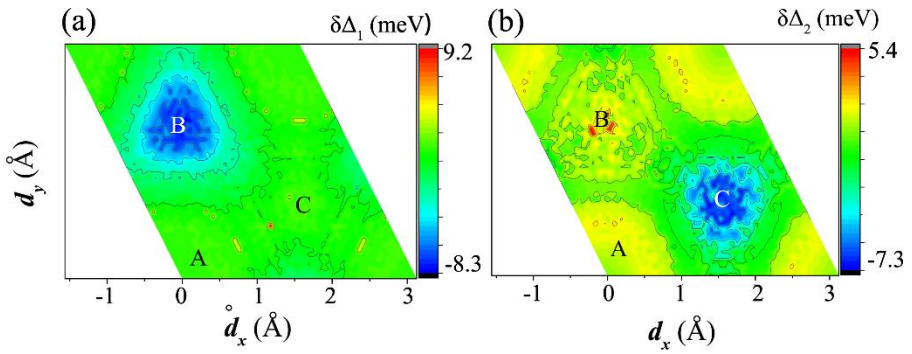

Figure S1. **Moiré modulated local intralayer gaps.** Variation of intralayer band gaps Δ_1 (a) and Δ_2 (b) as a function of $\boldsymbol{d}$.

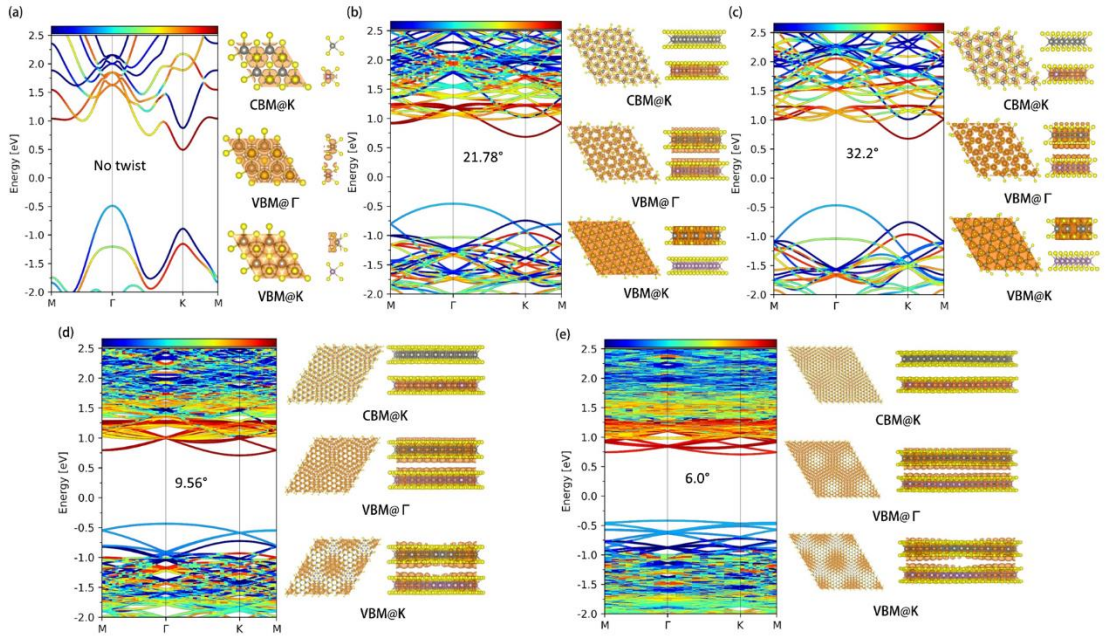

Figure S2. **Twist angle dependent electronic structures.** Band structures and charge densities of VBM and CBM for MoS_2/WS_2 heterostructures with different twist angles.

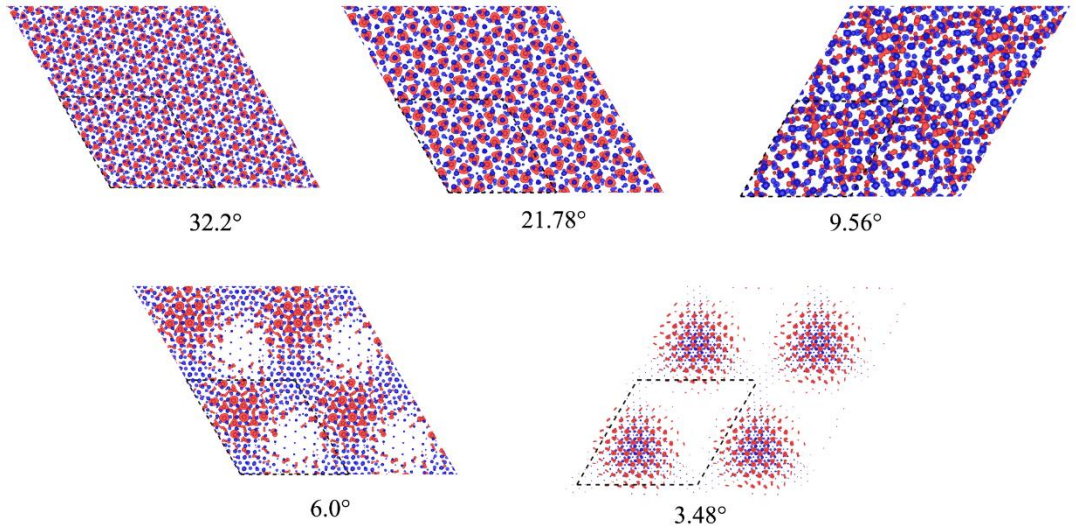

Figure S3. **Exciton charge densities of MoS_2/WS_2 heterostructures with different twist angles.**

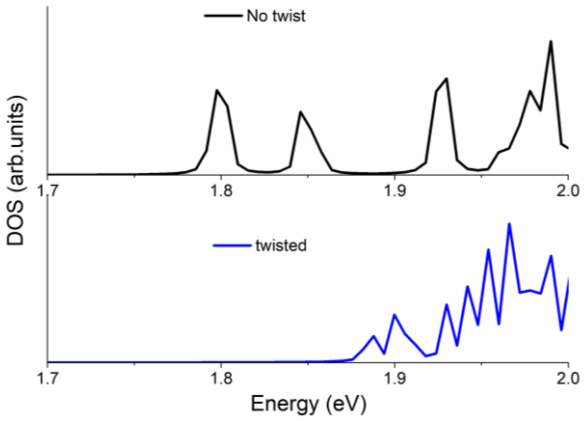

Figure S4. **Exciton energy splitting by moiré potential.** Excitonic density of states (DOS) for MoS_2/WS_2 heterostructures with $\theta=0°$ (no twist) and $\theta=3.48°$. The DOS of twisted heterostructure shows denser energy spacing.

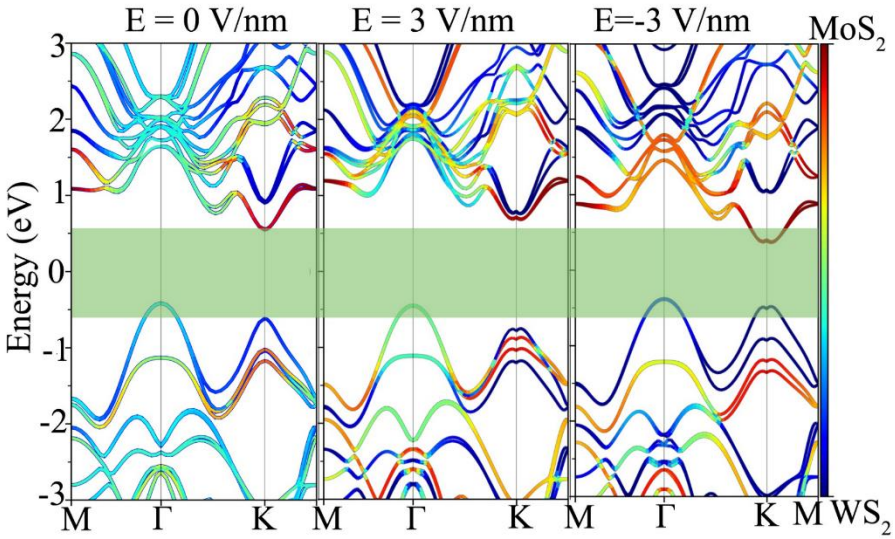

Figure S5. **Band structure of MoS_2/WS_2 heterostructure ($\theta=0°$) under electric field**. PBE+SOC band structures of MoS_2/WS_2 heterostructure ($\theta=0°$) under different electric fields, showing the energy level shifts that are consistent with Figure 6(a).