Supporting Information

Electronic structural Moiré pattern effects on $MoS_2/MoSe_2$ 2D heterostructures

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1. The band structure calculations from VASP and PEtot

The band structures of I^A and III^A obtained from VASP and PEtot (upon which the LS3DF method is based) are plotted in Fig. S1. Both calculations include spin-orbit coupling. The general feature is very similar. The band gaps are direct, with the CBM and VBM located at the K point. The band gaps calculated from VASP and PEtot for all the small systems considered are listed in Tab. S1. The trends of the band gap using these two packages are also very similar. The PEtot calculated gap is only 0.02~0.03 eV larger than that obtained by VASP.

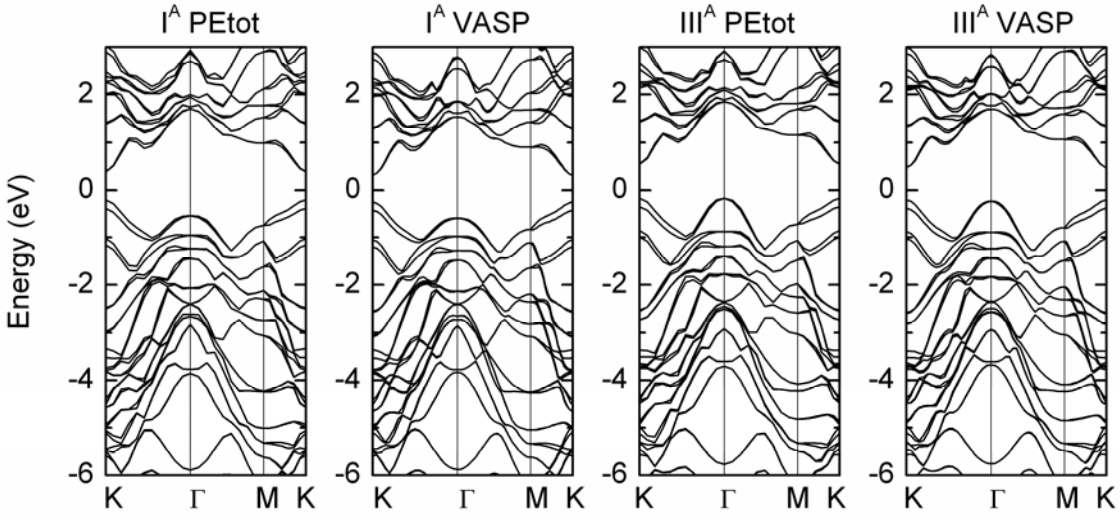

Fig. S1. The band structures of IA and IIIA obtained from VASP and PEtot.

Tab. S1. The band gaps calculated from VASP and PEtot for all the small systems considered.

	I^A	II^A	III^A	IV^A	V^A	VI^A	I^B	II^B	III^B	IV^B	V^B	VI^B
E_g-PEtot(eV)	0.59	0.63	0.72	0.64	0.59	0.61	0.66	0.62	0.60	0.62	0.65	0.64
E_g-VASP(eV)	0.57	0.60	0.69	0.62	0.57	0.58	0.63	0.60	0.57	0.59	0.62	0.61

2. Estimated errors induced by interpolation scheme

To test our interpolation scheme for the atomic displacement when constructing the Moiré structure, we have calculated a small system (latticed matched) between I^A and II^A (the same has been tested for that between II^A and III^A). For such a small system, we can get the vertical displacement using the interpolation scheme, or using direct DFT relaxations. We found the DFT relaxed inter-layer distance is 3.68 Å, while the interpolation gives 3.63 Å, thus the error is about 0.05 Å (while the overall vertical displacement is about 0.7 Å). Furthermore, the absolute eigenenergy error (due to the interpolation displacement error) relative to the vacuum level is only 1~2 meV for C1 and V1 stsates, and ~15 meV for V2 state. Thus, the electronic structure error due to the displacement interpolation scheme is small.

3. Moiré patterns with different relative orientations of the two layers

Fig. S2 shows Moiré patterns with different relative orientations of the two layers, with their natural mismatched lattice constants.. When the angle θ of crystallographic axes of the two atomic layers increases from 0 degree to 30 degrees, the size of the pattern becomes smaller. In the 30-degree case, the pattern becomes complex and the electronic structure is probably very different from the small angle cases. Nevertheless, in the cases of small θ (e.g., $\theta < 10$ degrees), the Moiré patterns are very similar, although the pattern sizes and scales are different. To demonstrate the same hole localization exist in these small angle cases, we have followed the same procedure as in the θ=0 case and calculated the VBM distribution of a 2-degree Moiré pattern case. The VBM wavefunction is shown in Fig.S3, it is clear that the same wavefunction localization exists. This does prove that the phenomenon is general and it doesn't need the exact orientation alignment between the MoS_2 layer and $MoSe_2$ layer.

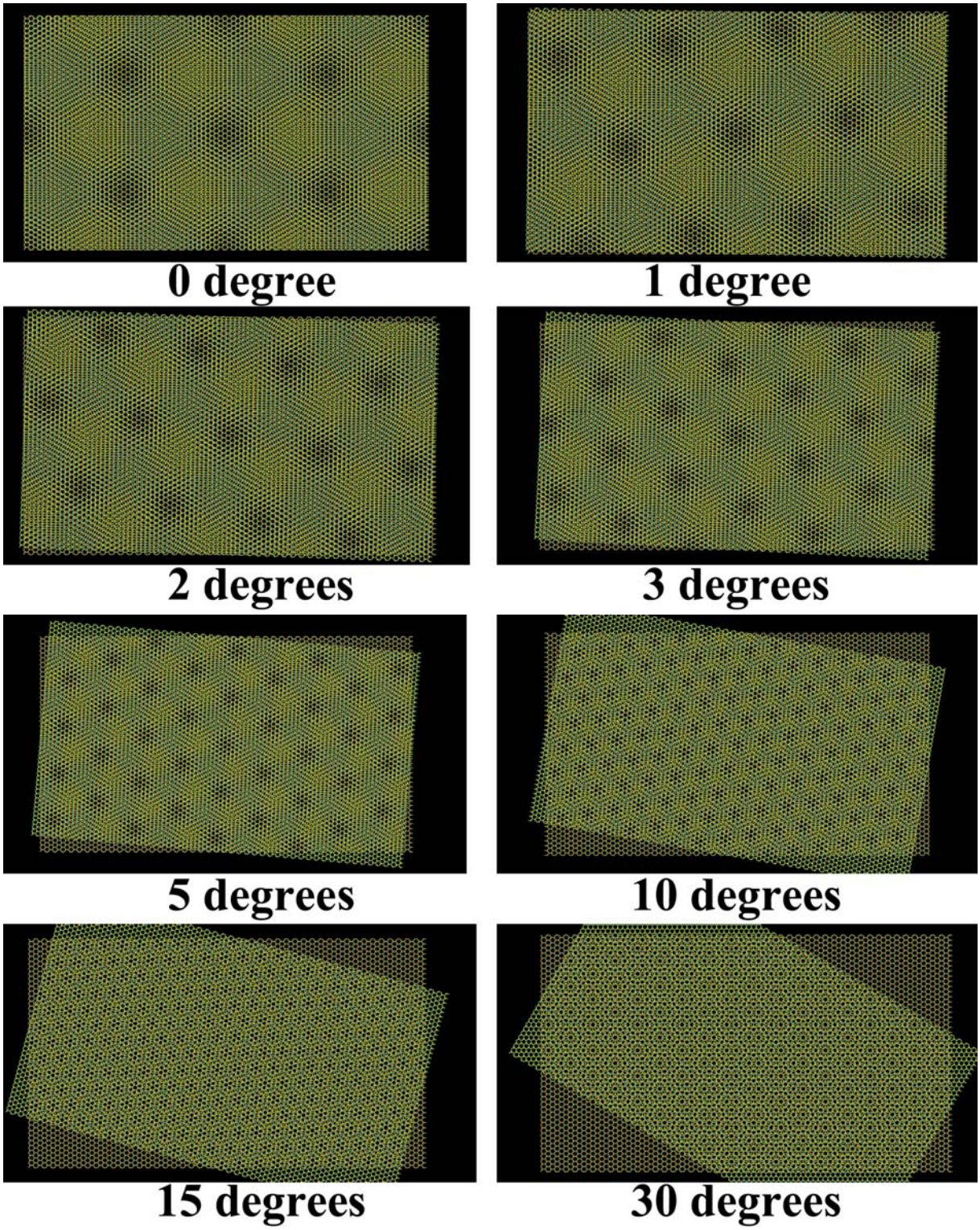

Fig. S2. Moiré patterns with different relative orientations of MoS_2 and $MoSe_2$ layers.

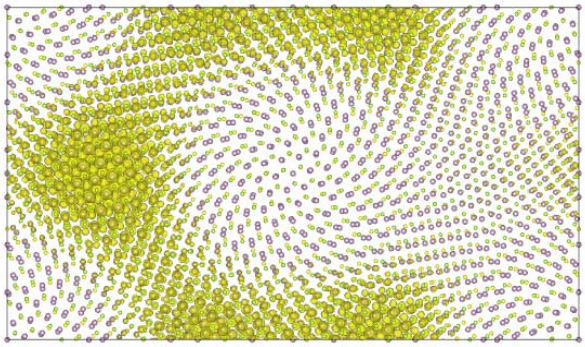

Fig. S3. The VBM distribution of a Moiré pattern with the MoS_2 layer rotated 2 degrees with respect to the $MoSe_2$ layers.