

Supporting Information:

Exciton Manipulation in Rippled Transition Metal Dichalcogenide

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1. The optical absorption spectrum

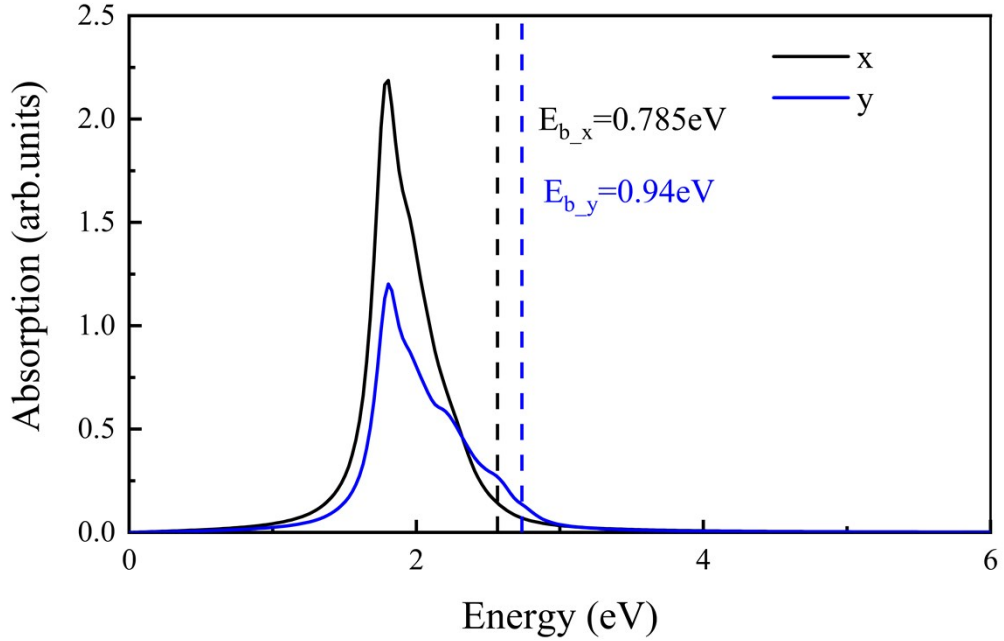


Figure S1. The calculated dielectric functions ϵ_2 for x-polarized (black solid line) and y-polarized (blue solid line) in SC-10. The GW bandgaps for first bright excitations are marked with vertical dash lines.

2. The effect of local strain on rippled MoS₂

As shown in **Table 1**, under the same compressive stress, the change of direct band gap is smaller in rippled MoS₂ monolayer compared to that in rippled MoSSe monolayer. After band folding, the K point of monolayer structure is folded to the 2/3 along Γ -X path (namely K' point) in rippled structure. As demonstrated in **Fig. 2**, the position of direct band gap is still kept at K' point in rippled MoS₂. In addition, similar to the case of flat MoS₂, the bright-to-dark transition is not observed in rippled MoS₂. The contribution of the first bright exciton in rippled MoS₂ is by the transition from the VBM to CBM at K' point, which is also the same as that in flat MoS₂. While for rippled MoSSe, the situation is quite different. The position of direct band gap no longer locates at K' point (namely A point as shown in **Fig. 2** of the manuscript) and varies with the variation of local strain. From the above, we come to the conclusion that non-uniform strain has less impact on rippled MoS₂ not only on electronic properties but also on optical properties.

3. The real-space distribution of excitation

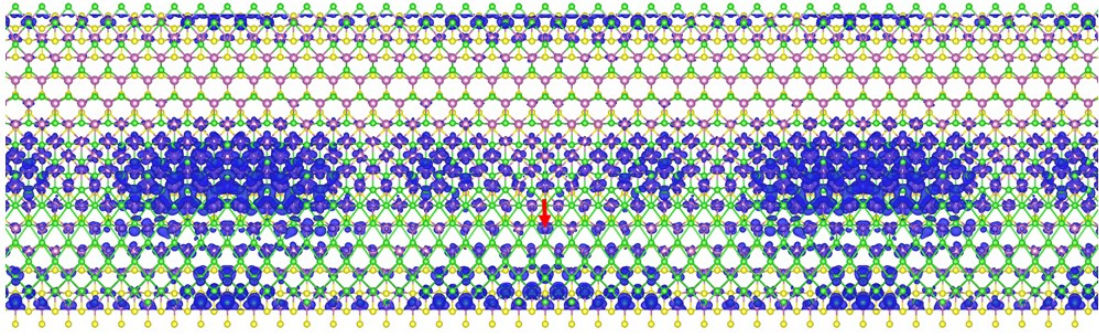


Figure S2. The Top views of real-space distribution of X_1 for y -polarized light in SC-10. The fixed hole position is indicated by red arrow.

4. The partial charge densities at CBM

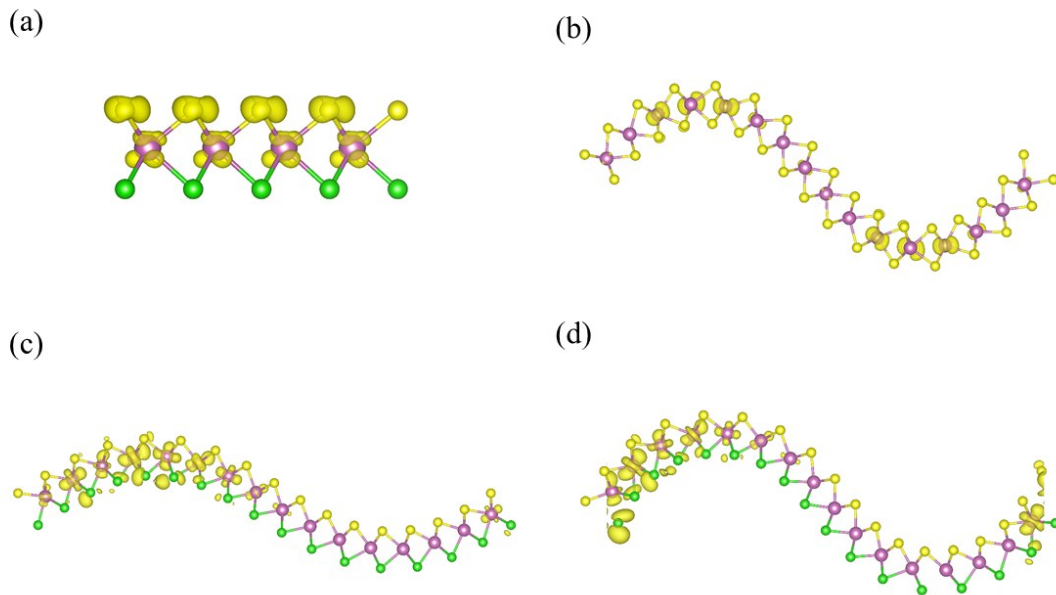


Figure S3. Top views of partial charge densities of (a) flat Janus-MoSSe, (b) rippled MoS₂, (c) SC-15, and (d) SC-10 for CBM at the k -points where make a major contribution to X_1 exciton.

5. The schematic diagram of X_0 and X_1 excitons of rippled MoSSe

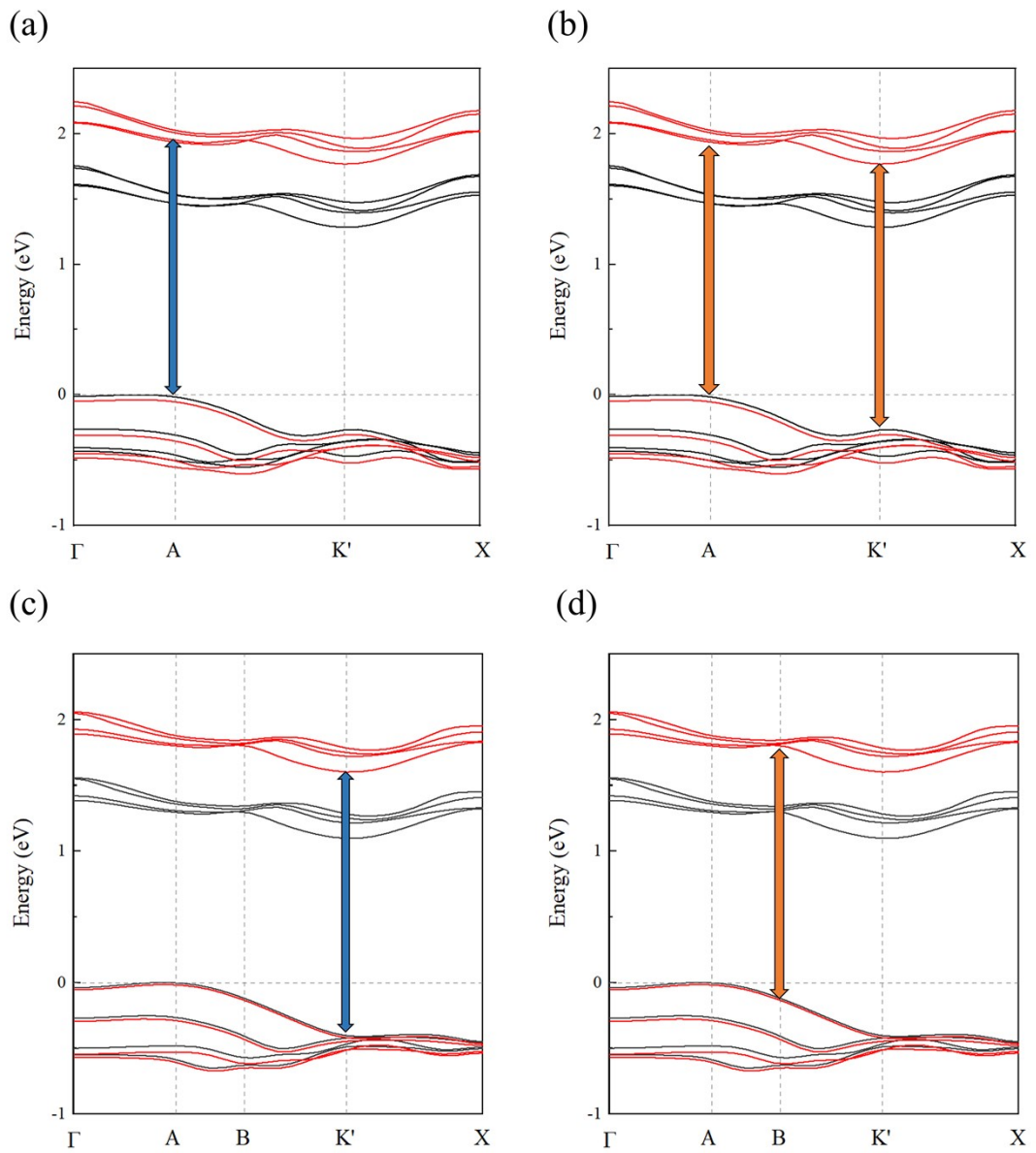


Figure S4. The schematic diagram of the contribution for (a) X_0 exciton and (b) X_1 exciton of SC-15 as well as (c) X_0 exciton and (d) X_1 exciton of SC-10. The blue and orange arrow point out the location where the transition takes place.