Supporting Information

of

Substrate mediated electronic and excitonic reconstruction in MoS_2 monolayer

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1. Effect of number of unoccupied bands on the optical spectra

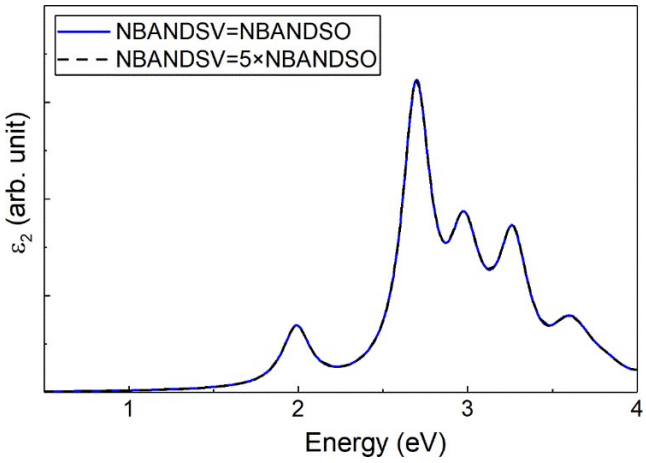

Figure S1. The optical spectra of MoS_2 monolayer calculated by same number of occupied states/unoccupied states (6 bands each), and the number (30 bands) of unoccupied states 5× the occupied states (6 bands).

To further validate BSE calculation accuracy of MoS_2 monolayer, we increased the number of unoccupied states to 5× the number of occupied states, and find that the difference of the first exciton peaks is unnoticeable, as shown in Figure S1

2. Effect of spin-orbital coupling on the exciton binding energy

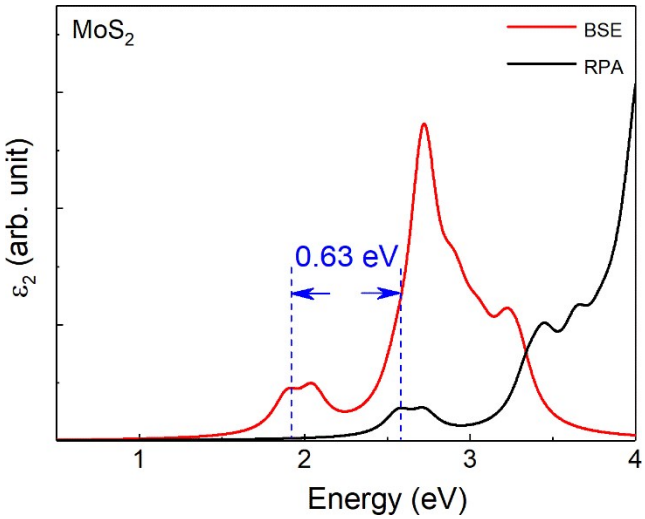

Figure S2. The optical spectra of MoS_2 monolayer with spin-orbit coupling effect calculated by BSE and RPA, respectively.

We have validated the SOC effect on the accuracy of our calculations by comparing the exciton binding energy of MoS_2 monolayers with/without the SOC. As Figure R2 shows, The effect of SOC on the exciton binding energy is within 0.02 eV.

3. Relative stability of MoS_2 monolayer on the substrates

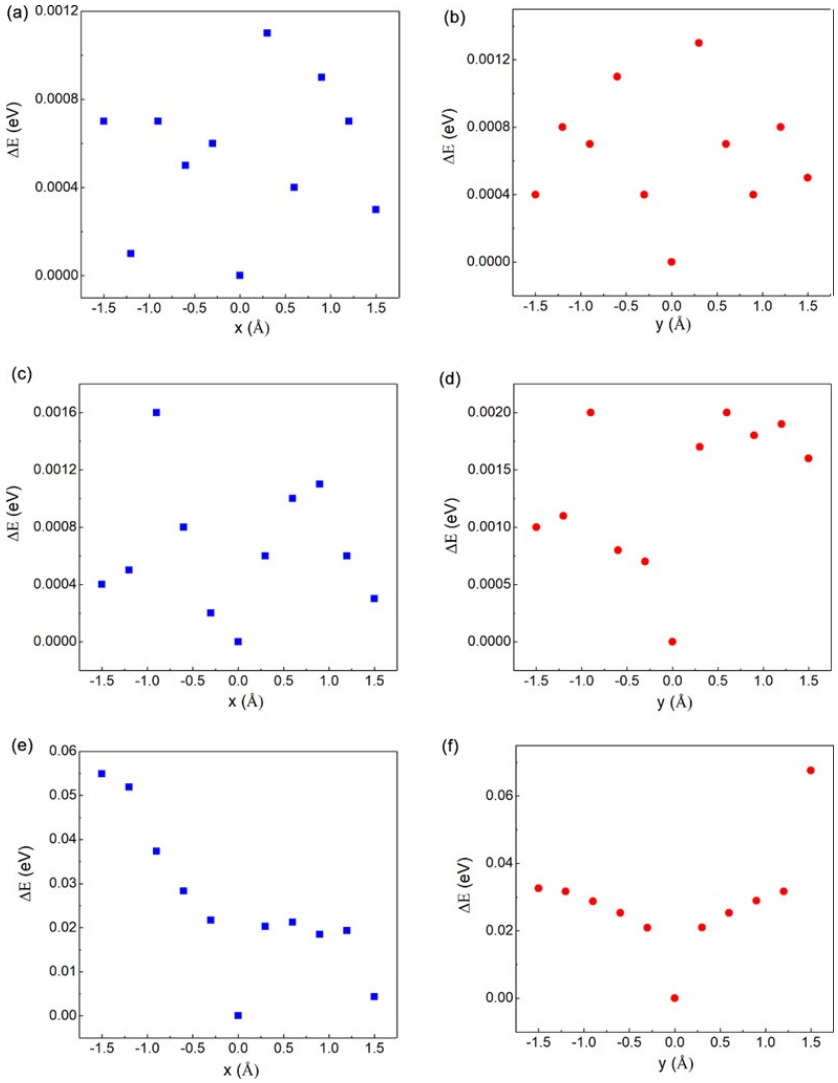

Figure S3. The relative stability of MoS_2 monolayer sliding on the substrates along x and y direction with a step of 0.3 Å. (a) and (b) MoS_2 on bi-layer graphene, (c) and (d) MoS_2 on bi-layer BN, and (e) and (f) MoS_2 on bi-layer GeC.

Figure S3 shows the energy difference of MoS_2 monolayer sliding on the substrates along x and y direction with a step of 0.3 Å. It can be seen that the energy difference of the various

configurations for MoS_2 monolayer on graphene bi-layer is small, within 1.5 meV. This suggests weak interaction between MoS_2 and graphene. The interaction between MoS_2 and h-BN is weak as the energy difference for their different configuration is also small, within 2 mV. In contrast, the energy difference is increased to several ten meV for various configurations of MoS_2 monolayer on the bi-layer GeC substrate, which suggests that the interaction between MoS_2 and GeC is stronger than that of MoS_2 on graphene and h-BN. All these results are consistent with the calculated adsorption energy.