Supporting Information
of
Substrate mediated electronic and excitonic reconstruction in MoS$_2$ monolayer

Yulin Yang$^1$, Tingting Song$^2$, Xiaoman Zhang$^3$, Yifei Zhao$^4$, Jingshan Chai$^5$, Zaijun Cheng$^1$, Xiaohua Huang$^1$, Hongyi Zhang$^1$,*, Wenzhang Zhu$^1$,*, and Ming Yang$^6$,*

$^1$ Fujian Provincial Key Laboratory of Optoelectronic Technology and Devices, School of Optoelectronic and Communication Engineering, Xiamen University of Technology, Xiamen, 361024, China

$^2$ College of Physics and Space Science, China West Normal University, Nanchong, 637002, China

$^3$ College of Photonic and Electronic Engineering, Fujian Normal University, Fuzhou, 35007, China

$^4$ School of Physics and Technology, Wuhan University, Wuhan, 430072, China

$^5$ Department of Polymer Science and Engineering, Zhejiang University, Zhe Da Road 38, Hangzhou 310027, China

$^6$ Institute of Materials Research and Engineering, Agency for Science, Technology and Research (A*STAR), 2 Fusionopolis Way, Innovis, 138634, Singapore

# These authors contributed equally to this work.

*Correspondence: M.Y (yangm@imre.a-star.edu.sg); H.Z (zanghongyi@xmut.edu.cn); W.Z. (wzzh@xmut.edu.cn)
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

![Graphs showing energy difference of MoS$_2$ monolayer sliding on substrates](image)

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.