Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

"Improved visible-light absorbance of monolayer MoS_2 on AlN substrate and angle-dependent electronic structures"

Feifei Li[2], Changmin Shi[1,*], Dongchao Wang[1], Guangliang Cui[1], Pinhua Zhang[1], Li Lv[1] and Li Chen[1]

[1]Institute of Condensed Matter Physics, School of Physics and Electric Engineering, Linyi University , Linyi 276000, China

[2]State-owned Assets and Laboratory Management, Linyi University, Linyi 276000, China

E-mail addresses: scm ff@163.com, shichangmin@lyu.edu.cn (C. M. Shi).

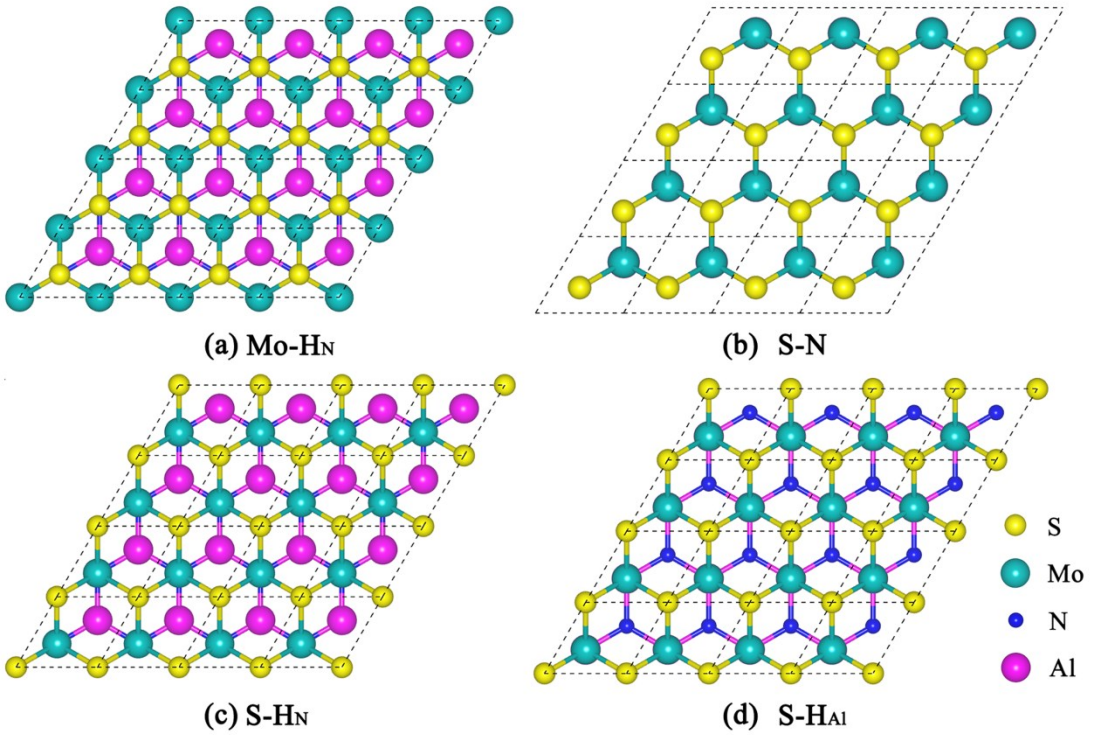

Fig. 1S The top views of (a) Mo-H_N, (b) S-N, (c) S-H_N and (d) S-H_{Al} stacked MoS_2/AlN hetero-structures with lattice match model.

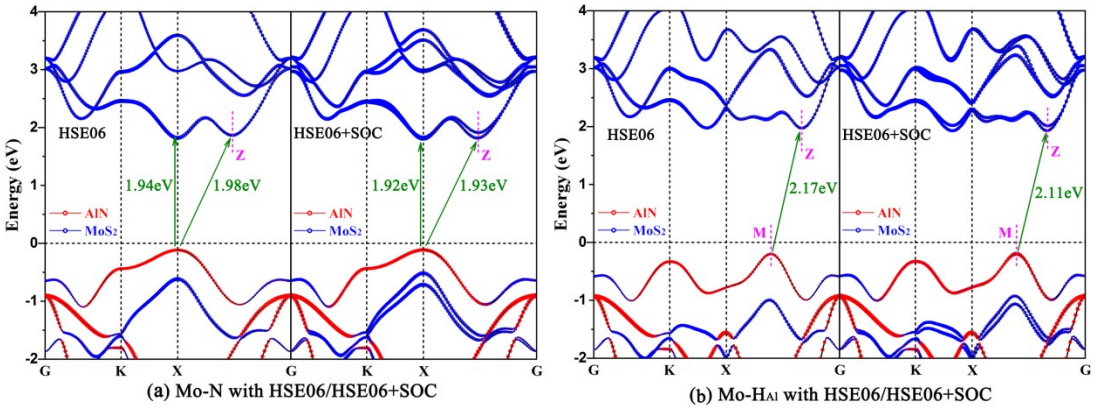

Fig. 2S The electronic band structures of (a) Mo-N and (b) Mo-H_N stacked hetero-structures with HSE06 and HSE06-SOC formations.

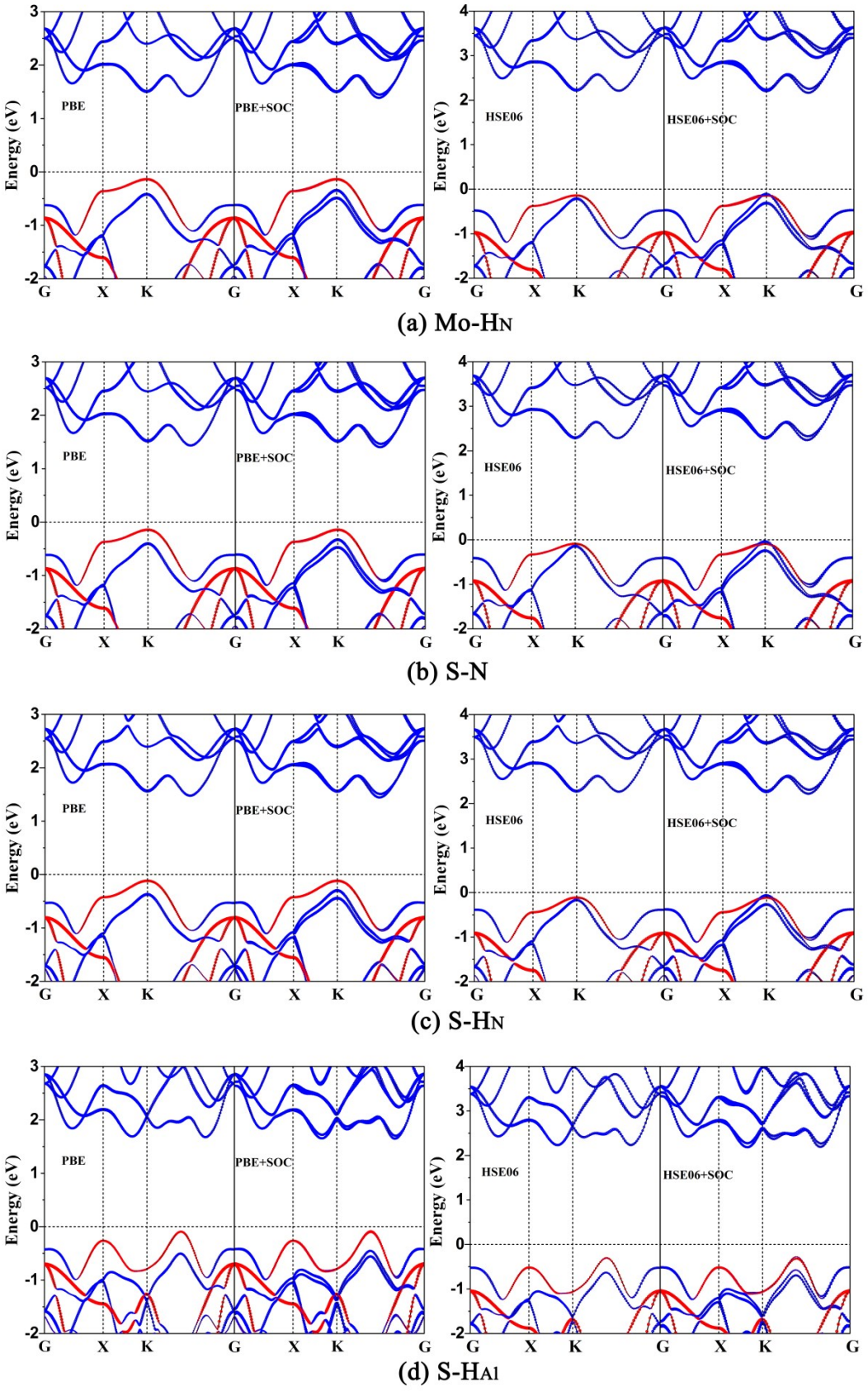

Fig. 3S The electronic band structures of (a) Mo-H_N, (b) S-N, (c) S-H_N and (d) S-H_{Al} stacked MoS_2/AlN hetero-structures with lattice match model.

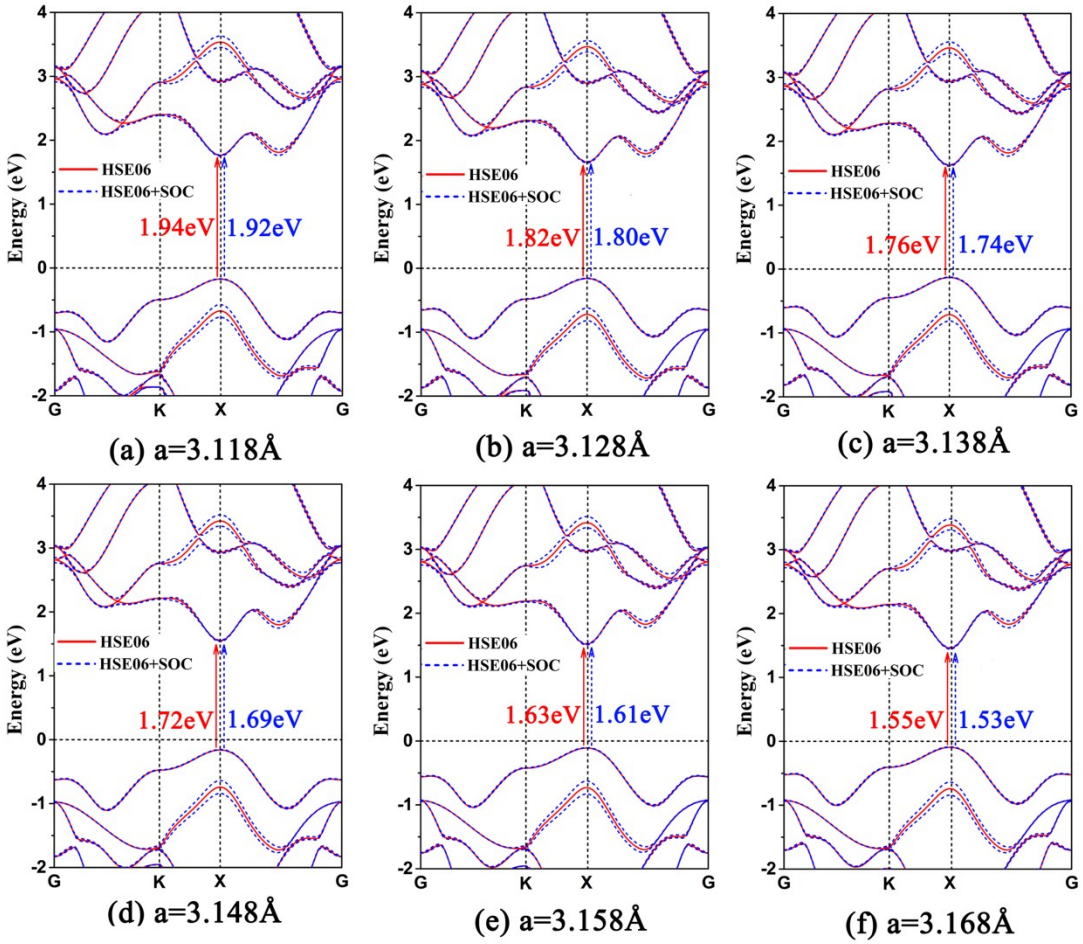

Fig. 4S The electronic band structures of MoS_2/AlN hetero-structures with HSE06 and HSE06-SOC formations in Mo-N stacking configurations for different lattice constants from a = 3.118Å to a = 3.168Å.

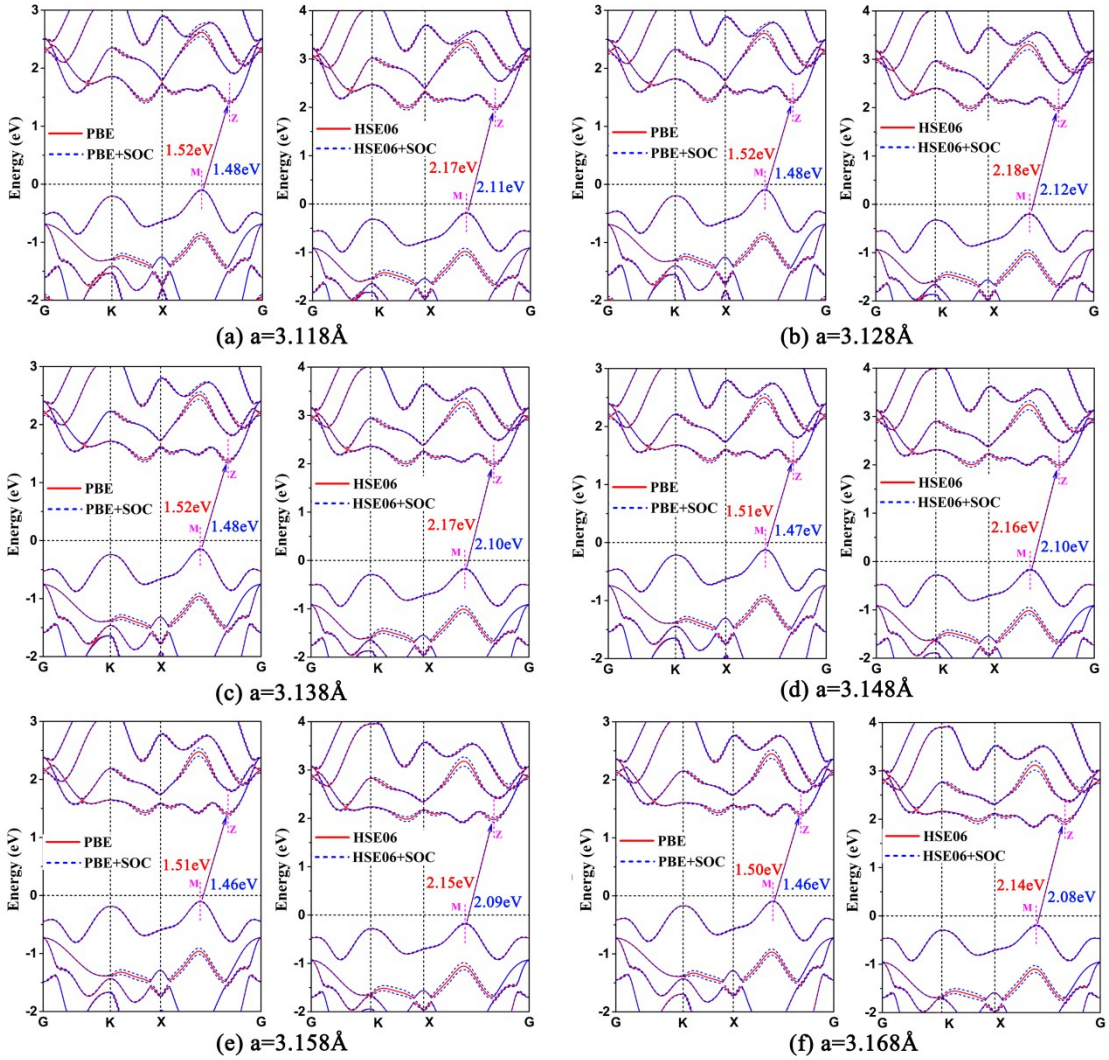

Fig. 5S The dependences of electronic band structures of Mo-H_{Al} stacked MoS_2/AlN hetero-structures on strains from a=3.118Å to a=3.168Å.

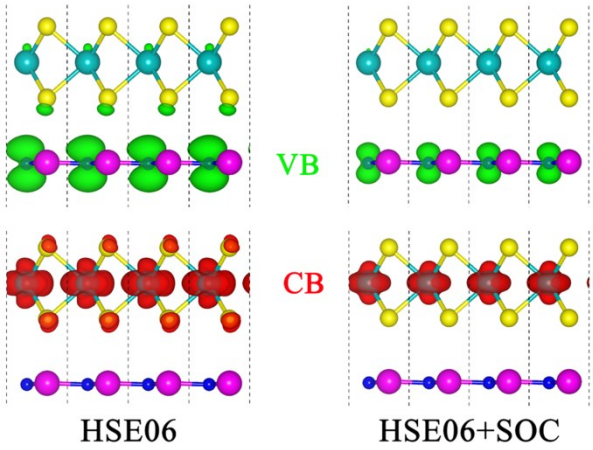

Fig. 6S The partial decomposed charge density of VB and CB of Mo-N stacked MoS_2/AlN hetero-structures with HSE06 and HSE06-SOC formations.

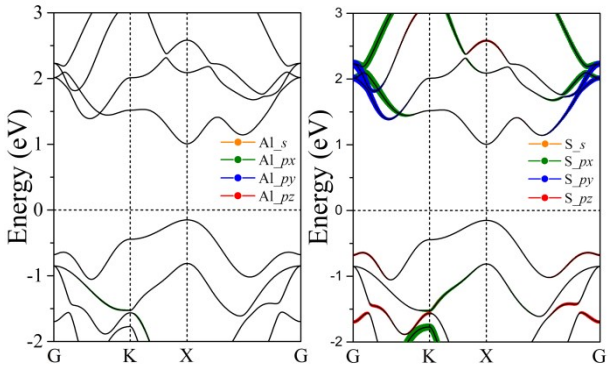

Fig. 7S The partial orbitals of (a) Al atoms with PBE formation and (b) S atoms with PBE formation.