Supplementary Information for

“Improved visible-light absorbance of monolayer MoS$_2$ on AlN substrate and angle-dependent electronic structures”

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Fig. 1S The top views of (a) Mo-H\textsubscript{N}, (b) S-N, (c) S-H\textsubscript{N} and (d) S-H\textsubscript{Al} stacked MoS\textsubscript{2}/AlN heterostructures with lattice match model.

Fig. 2S The electronic band structures of (a) Mo-N and (b) Mo-H\textsubscript{N} stacked hetero-structures with HSE06 and HSE06-SOC formations.
Fig. 3S The electronic band structures of (a) Mo-HN, (b) S-N, (c) S-HN and (d) S-HAl 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 $a = 3.118\,\text{Å}$ to $a = 3.168\,\text{Å}$. 
Fig. 5S The dependences of electronic band structures of Mo-H\textsubscript{Al} stacked MoS\textsubscript{2}/AlN heterostructures 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\textsubscript{2}/AlN heterostructures 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.