Electronic Supplementary Information

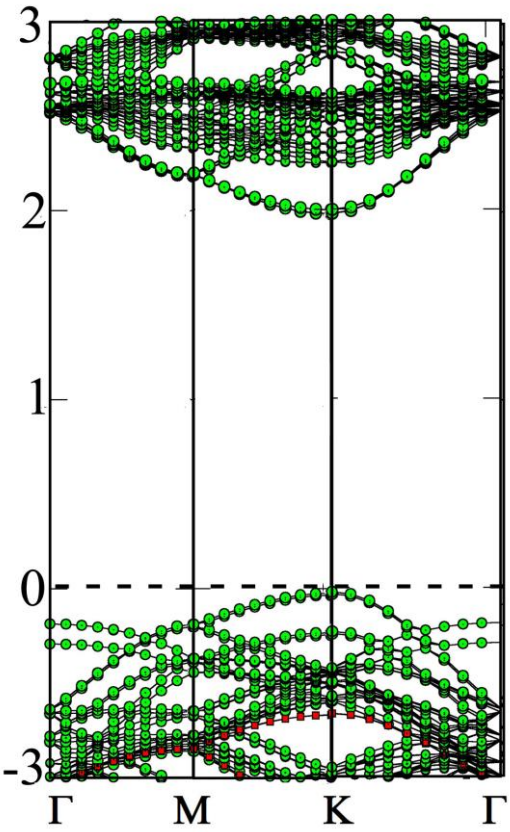

Figure S1. The HSE06 band structure of MoS_2/BN/MoS_2 trilayer with the A1B1A1 stacking. The green lines represent MoS_2 layers while the red lines represent BN layer.

Table S1.The optimized cell parameter a_1 (in Å) of MoS_2/ML/MoS_2 trilayer, the distance d_1 (in Å) between two nearest-neighbor monolayers of MoS_2/ML/MoS_2 trilayer, the charge transfer **Δe** (in electron) from ML to MoS_2 layers per unit cell, the optimized cell parameter a_2 (in Å) of MoS_2/ML superlattice layers, the binding energy E_{BE1} (in eV) of MoS_2/ML/MoS_2 hetero-layers, and the binding energy E_{BE2} (in eV) of MoS_2/ML superlattice layers.

	$MoSe_2$ (ABA)	**$MoSe_2$ (ACA)**	**WS_2 (ACA)**	**WS_2 (ACA)**	**WSe_2 (ABA)**	**WSe_2 (ACA)**
a_1	3.24	3.24	3.19	3.19	3.24	3.24
d_1	3.18	3.13	3.13	3.13	3.14	3.19
Δe	0.02	0.02	0	0	0.02	0.02
a_2	3.26/12.82	3.26/12.72	3.19/12.49	2.19/12.42	3.26/12.82	3.26/12.76

E_{BE1}	0.36	0.36	0.45	0.45	0.36	0.36
E_{BE2}	0.39	0.40	0.45	0.45	0.40	0.40

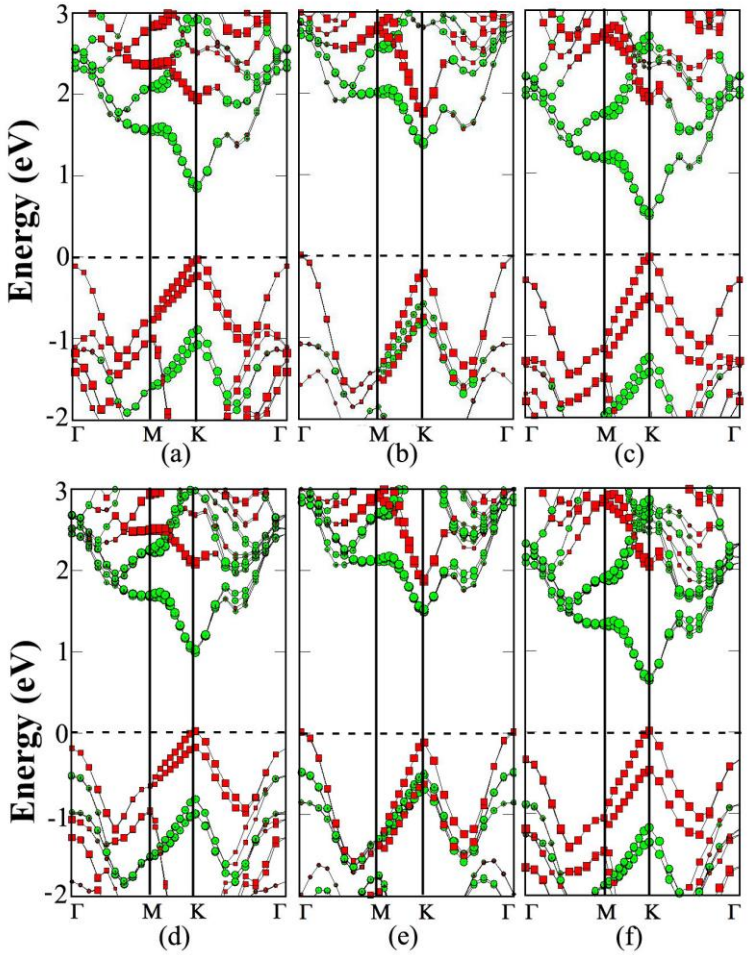

Figure S2. The HSE06 band structures of (a) $MoS_2/MoSe_2/MoS_2$ (b) $MoS_2/WS_2/MoS_2$ (c) $MoS_2/WSe_2/MoS_2$ trilayers with ABA stacking, respectively. The HSE06 band structures of (d) $MoS_2/MoSe_2$ superlattice, (e) MoS_2/WS_2 superlattice, and (f) MoS_2/WSe_2 superlattice all with AB stacking, respectively.