Electronic Supplementary Material (ESI) for RSC Advances.


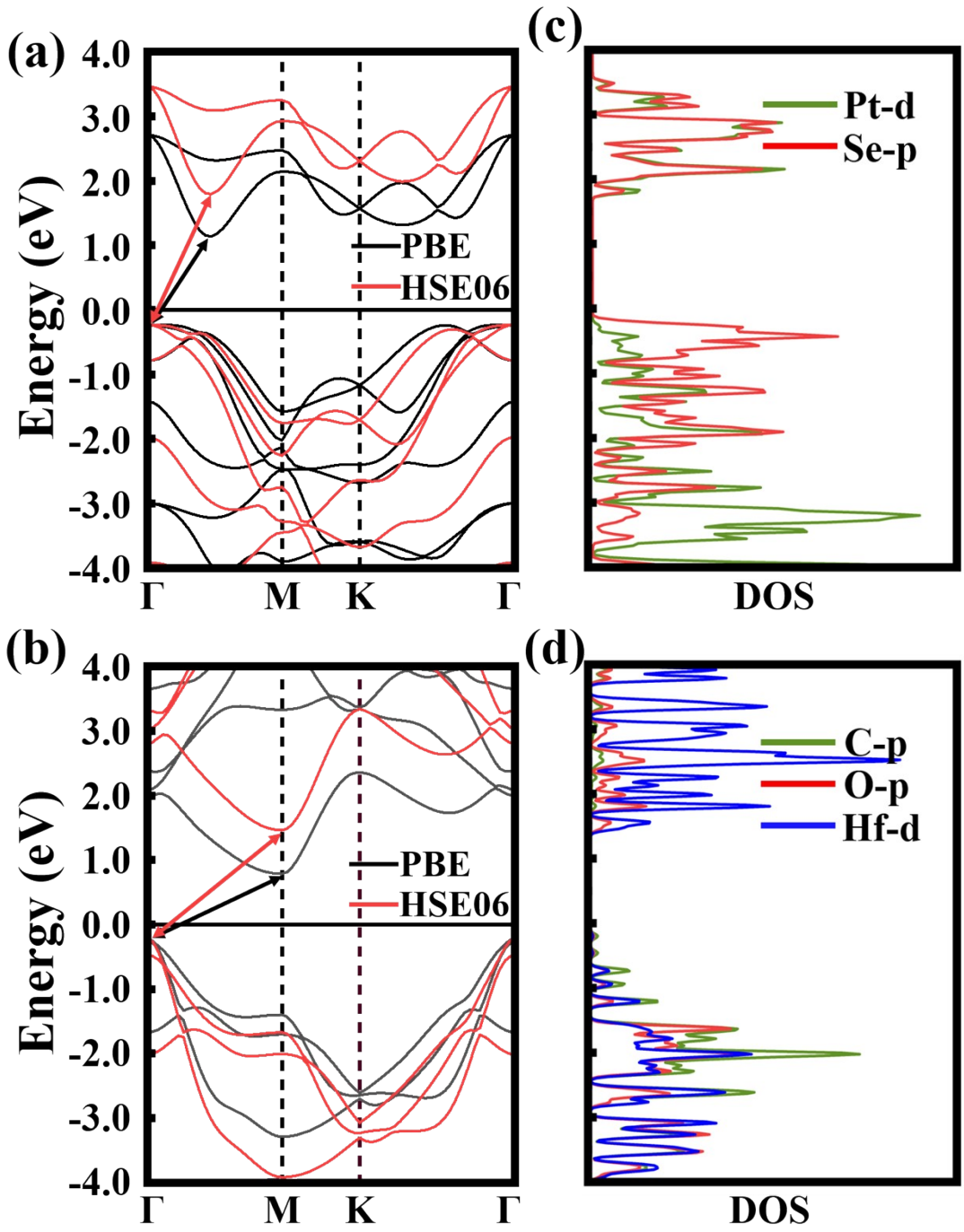


Fig.S1 (a,b) The band structures and (c,d) corresponding partial densities of states (PDOS) of the primitive cells of $PtSe_2$ and $Hf_2CO_2$ monolayers. The band structures are calculated by PBE & HSE06 methods, while the partial densities of states are calculated by HSE06 method with Fermi level is set to be zero, which are presented by black & red line, respectively.

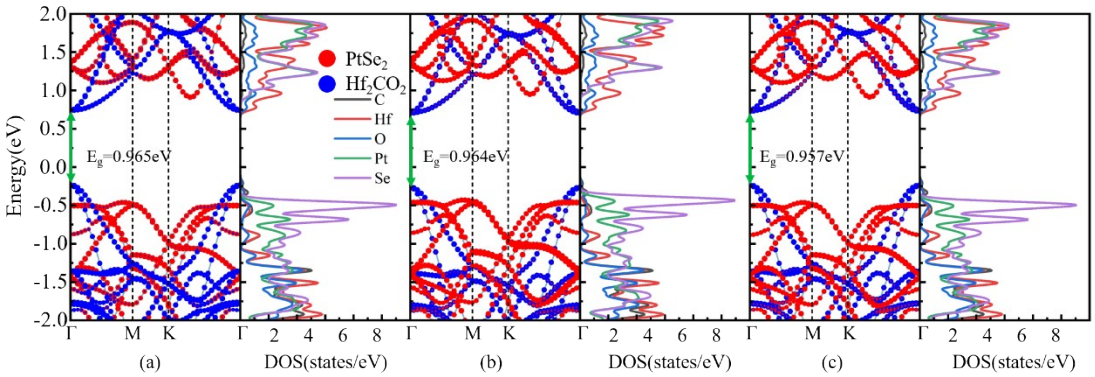


Fig.S2 The projected band structure and PDOS calculated by PBE functional of $PtSe_2/Hf_2CO_2$ vdW heterostructure with different stacks of (a) Stacking-I, (b) Stacking-II and (c) Stacking-III, respectively. The red and blue lines and dots represent are for $PtSe_2$ and $Hf_2CO_2$, respectively. The Fermi level is set at zero.

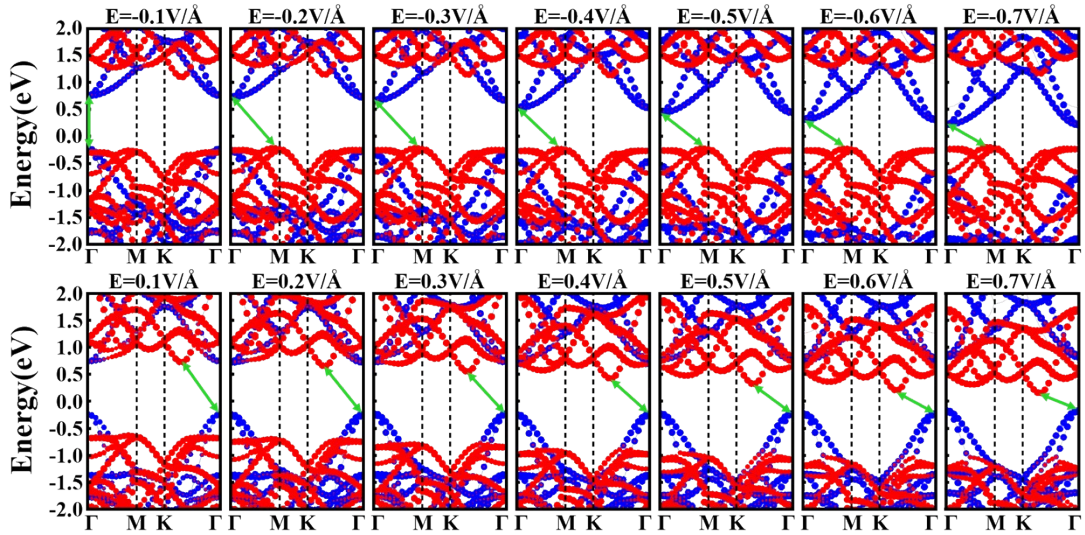


Fig.S3 The band structures of $PtSe_2/Hf_2CO_2$ heterostructure under the negative electric field varying from -0.1 to -0.7 V/Å, and positive electric fields varying from 0.1 to 0.7 V/Å, where the red and blue dots represent $PtSe_2$ and $Hf_2CO_2$, respectively. The green arrow lines represent the CBM and VBM.