Support Information

First-principles study on optoelectronic properties of Cs_2PbX_4-$PtSe_2$ van der Waals Heterostructures

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There are one table and three figures in Supplementary Material. Table S1 and Fig. S2 illustrate the band gap of monolayer Cs_2PbX_4 and $PtSe_2$ with different calculation functional. The unit cells of 2D Cs_2PbX_4-$PtSe_2$ are shown in Fig. S1. We computed the band structures of orbital contribution for Cs_2PbX_4-$PtSe_2$ heterostructures, as shown in Fig. S3.

Table S1 The bandgaps of monolayer Cs_2PbX_4 and $PtSe_2$ by different calculation method.

	Cs_2PbCl_4	Cs_2PbBr_4	Cs_2PbI_4	$PtSe_2$
PBE	2.59	2.18	1.84	1.38
HSE	3.58	2.91	2.57	1.96
PBE+SOC	1.84	1.46	1.09	1.21
HSE+SOC	2.78	2.14	1.78	1.79
expriment	3.01	2.32	1.86	1.20

*Exprimental values are from Ref. [6,14,25,45]

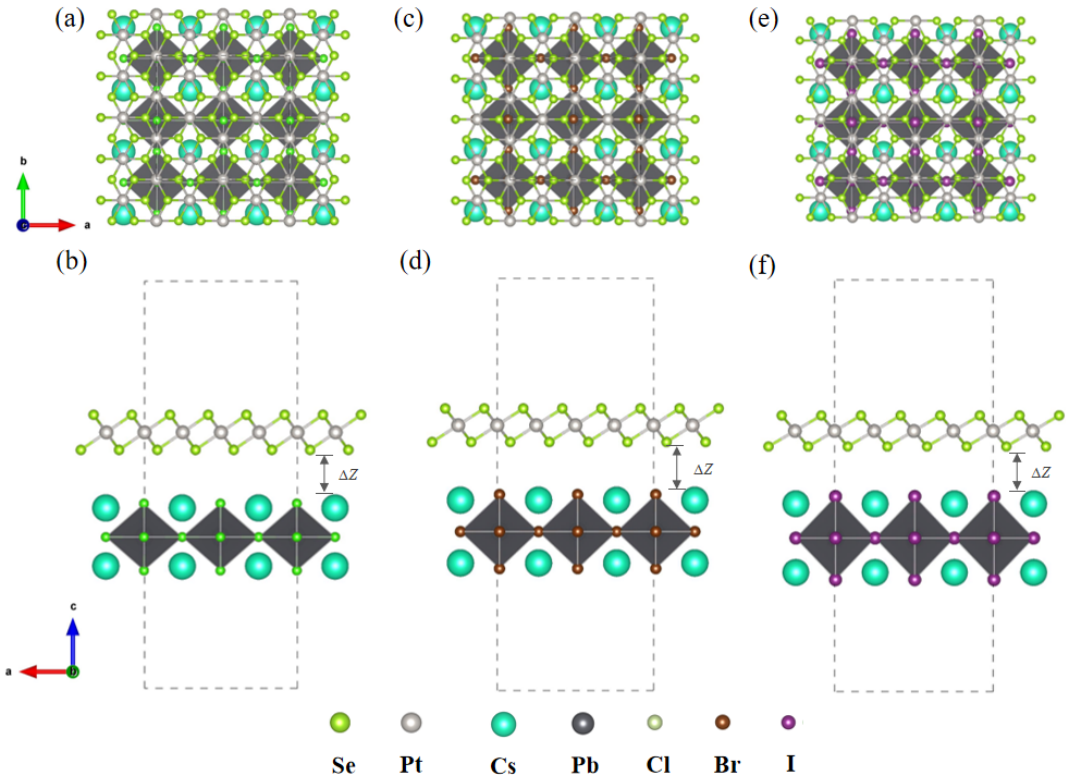

Fig. S1 Top and side views of relaxed 90° Cs_2PbX_4-$PtSe_2$ heterostructures. (a-b) Cs_2PbCl_4-$PtSe_2$ heterostructure. (c-d) Cs_2PbBr_4-$PtSe_2$ heterostructure. (e-f) Cs_2PbI_4-$PtSe_2$ heterostructure.

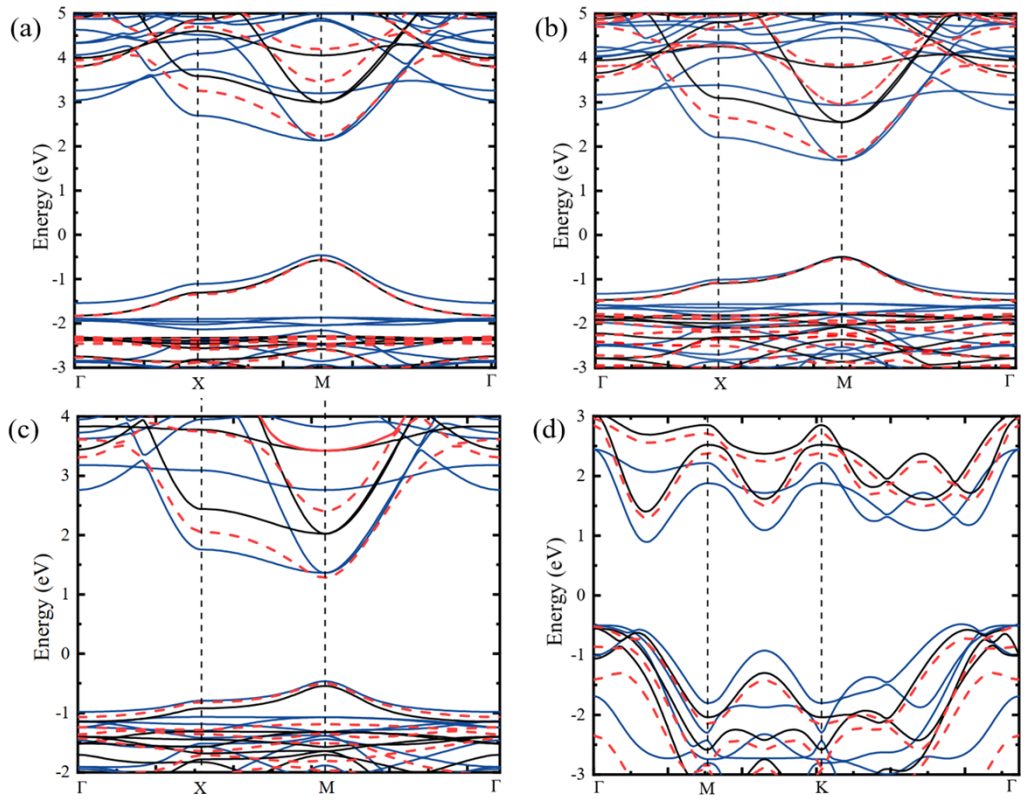

Fig. S2 The bandgaps of monolayer (a)Cs_2PbCl_4, (b)Cs_2PbBr_4, (c)Cs_2PbI_4, and (d) $PtSe_2$ by PBE, HSE and HSE with SOC. The blue, black and red lines correspond to PBE, HSE and HSE with SOC, respectively

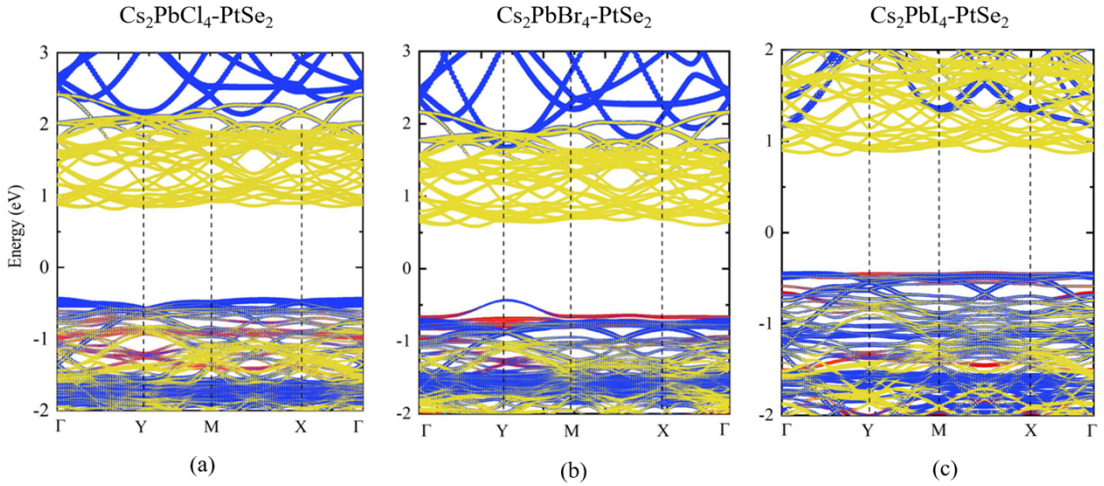

Fig. S3 The band structures of orbital contribution for Cs_2PbX_4-$PtSe_2$ heterostructures. The $p_{x,y}$-orbital, p_z-orbital and d-orbital contributions are indicated by blue, red and yellow dots, respectively.