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Electronic supplementary information for

Electronic structures and photovoltaic application of vdW heterostructure based-on Janus group-IV monochalcogenides: insight from first-principles calculations

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Table S1. The relaxed-ion elastic coefficients (C_{11}, C_{12}, C_{22}, and C_{44}) of four Janus group-IV monochalcogenides.

	C_{11} (N/m)	C_{22} (N/m)	C_{12} (N/m)	C_{44} (N/m)
$GeSnS_2$	39.58	15.43	18.29	18.21
$GeSnSe_2$	42.18	20.66	18.66	19.46
Ge_2SSe	45.02	15.27	19.88	20.88
Sn_2SSe	40.81	20.88	18.15	19.04

Table S2. Information of all 32 heterostructures: mismatch along zig-zag and air-chair direction (Δ_{mis}), band alignment at Anderson limit calculated with HSE06 functional, and power conversion efficiency of type II heterostructures.

	Δ_{mis}(%)		Type	PCE(%)
	Zig-zag	Arm-chair		
GeSe/$GeSnS_2$-Ge	2.87	2.94	II	18.07
GeSe/$GeSnS_2$-Sn			I	-
GeSe/$GeSnSe_2$-Ge	3.28	3.59	II	16.72
GeSe/$GeSnSe_2$-Sn			II	20.86
GeSe/Ge_2SSe-S	3.52	1.91	I	-
GeSe/Ge_2SSe-Se			I	-
GeSe/Sn_2SSe-S	4.75	2.90	II	19.19
GeSe/Sn_2SSe-Se			II	19.81
SnS/$GeSnS_2$-Ge	4.96	1.82	II	11.86
SnS/$GeSnS_2$-Sn			I	-
SnS/$GeSnSe_2$-Ge	1.20	2.46	II	11.20
SnS/$GeSnSe_2$-Sn			I	-
SnS/Sn_2SSe-S	2.66	1.77	I	-
SnS/Sn_2SSe-Se			I	-
SnSe/$GeSnSe_2$-Ge	3.99	0.52	II	16.40
SnSe/$GeSnSe_2$-Sn			I	-
SnSe/Sn_2SSe-S	2.53	0.16	I	-
SnSe/Sn_2SSe-Se			I	-
GeS/$GeSnS_2$-Ge	5.92	2.75	I	-
GeS/$GeSnS_2$-Sn			II	15.86
GeS/$GeSnSe_2$-Ge	12.06	2.11	I	-
GeS/$GeSnSe_2$-Sn			I	-
GeS/Ge_2SSe-S	5.28	3.78	II	17.48
GeS/Ge_2SSe-Se			II	17.88
GeS/Sn_2SSe-S	13.53	2.79	II	20.72
GeS/Sn_2SSe-Se			II	21.31
SnS/Ge_2SSe-S	5.60	0.78	I	-
SnS/Ge_2SSe-Se			II	16.74
SnSe/$GeSnS_2$-Ge	10.14	0.11	II	18.47
SnSe/$GeSnS_2$-Sn			I	-
SnSe/Ge_2SSe-S	10.78	1.15	I	-
SnSe/Ge_2SSe-Se			I	-

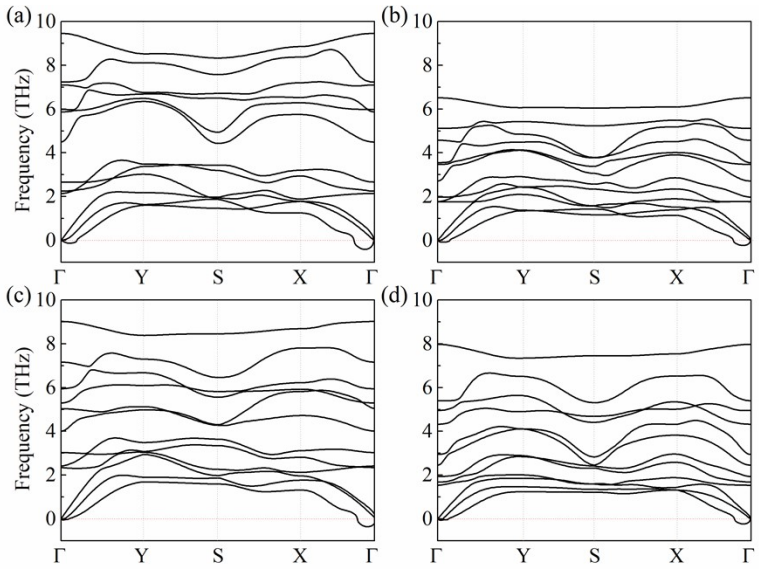

Fig. S1 Phonon dispersions of Janus (a) $GeSnS_2$, (b) $GeSnSe_2$, (c) Ge_2SSe, and (d) Sn_2SSe.

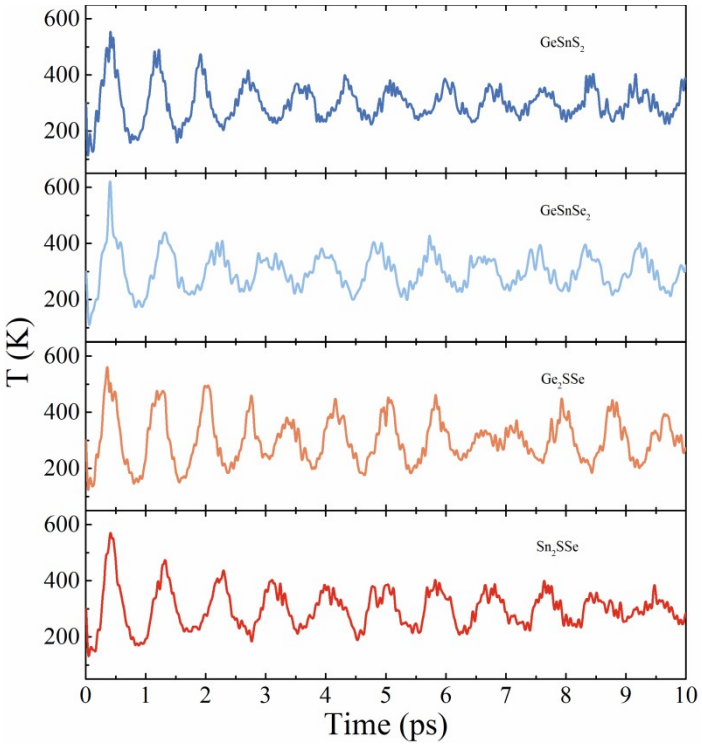

Fig. S2 Time evolution of temperature at each Janus group-IV monochalcogenides.

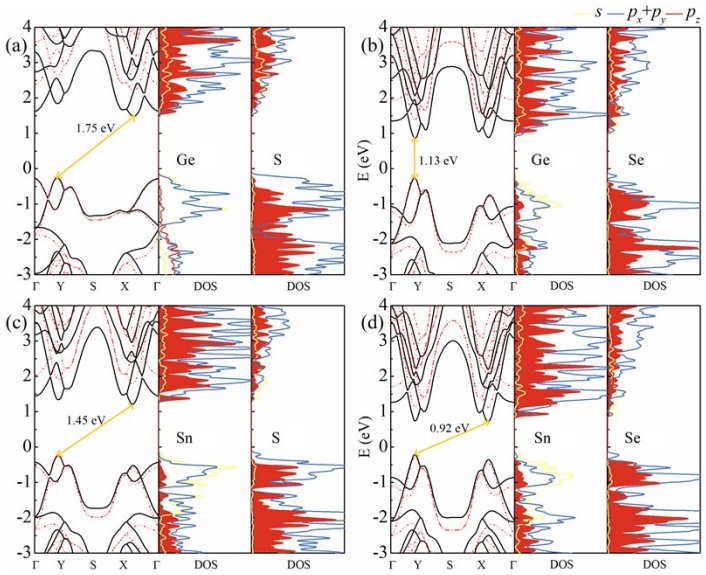

Fig. S3 Electronic band structures and partial density of states (DOS) of (a) GeS, (b) GeSe, (c) SnSe, and (d) SnSe. The black plots and the red dashed plots are calculated with PBE and HSE06 functional, respectively.

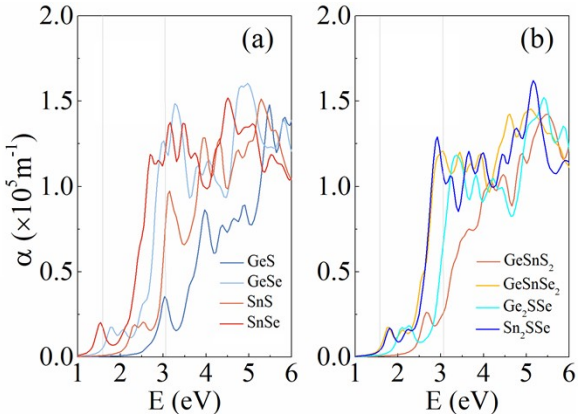

Fig. S4 Optical absorption spectrum of (a) pristine and (b) Janus group-IV monochalcogenides calculated with HSE06 functional. The two grey dashed lines denote the visible light region.

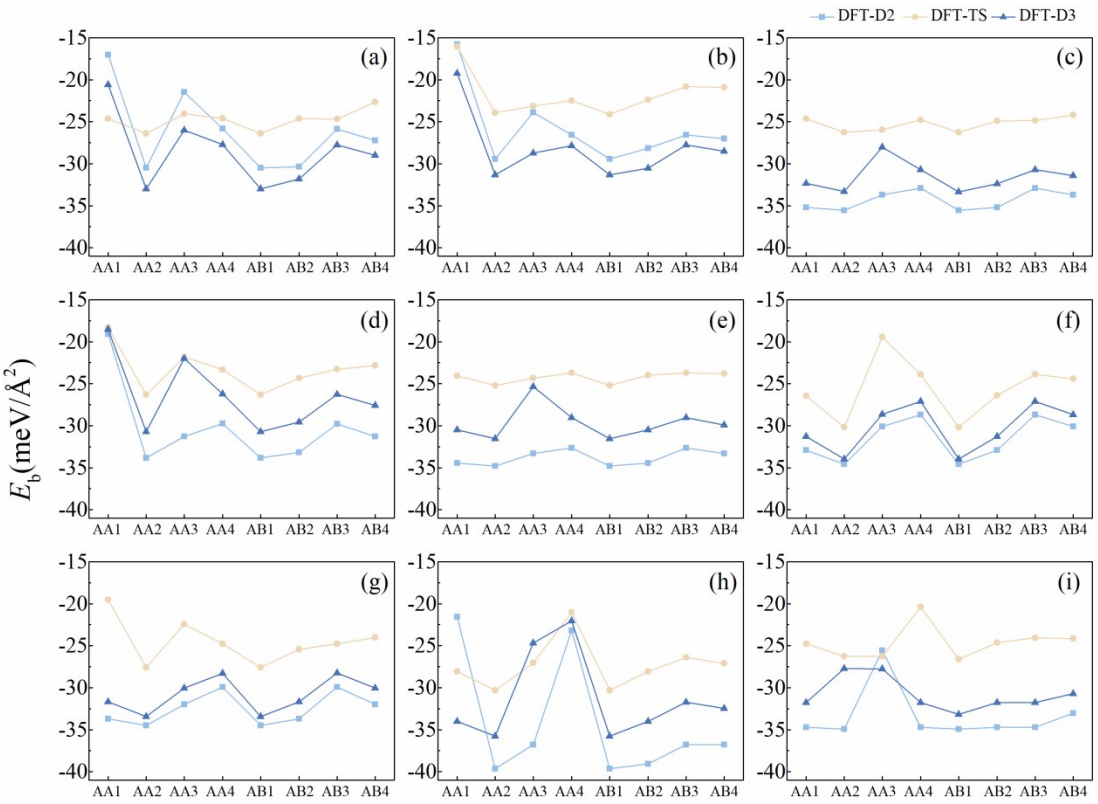

Fig. S5 Binding energy of eight stacking configurations at (a) GeSe/GeSnS$_2$-Ge, (b) GeSe/GeSnSe$_2$-Ge, (c) GeSe/GeSnSe$_2$-Sn, (d) GeSe/Sn$_2$SSe-S, (e) GeSe/Sn$_2$SSe-Se, (f) SnS/GeSnS$_2$-Ge, (g) SnS/GeSnSe$_2$-Ge, (h) SnS/GeSnSe$_2$-Sn and (i) SnSe/GeSnSe$_2$-Ge heterostructure calculated with DFT-D2, DFT-TS and DFT-D3 vdW dispersion correction.

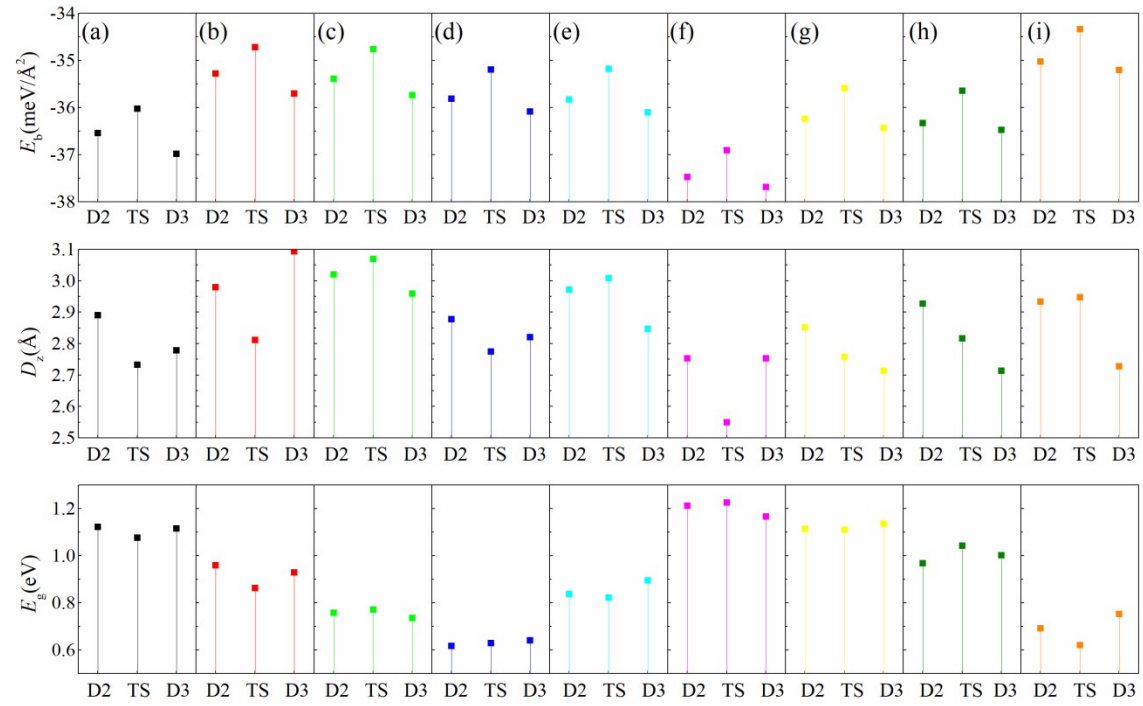

Fig. S6 Binding energy (upper), average vertical distance (middle), and band gap (lower) at (a) GeSe/$GeSnS_2$-Ge, (b) GeSe/$GeSnSe_2$-Ge, (c) GeSe/$GeSnSe_2$-Sn, (d) GeSe/Sn_2SSe-S, (e) GeSe/Sn_2SSe-Se, (f) SnS/$GeSnS_2$-Ge, (g) SnS/$GeSnSe_2$-Ge, (h) SnS/$GeSnSe_2$-Sn, and (i) SnSe/$GeSnSe_2$-Ge heterostructure of AB1 stacking configuration calculated with DFT-D2, DFT-TS, and DFT-D3 vdW dispersion correction.

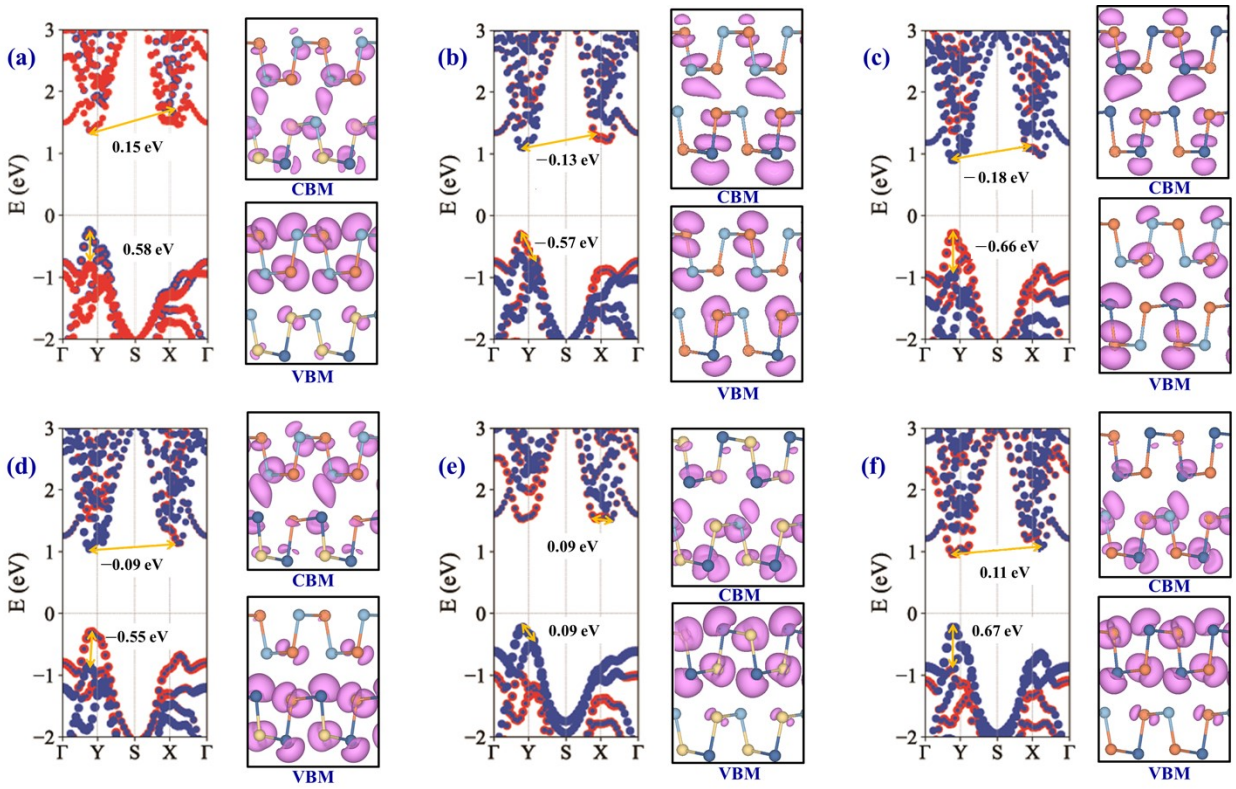

Fig. S7 Projected electronic band structures (left panel), the partial charge density of VBM (right lower panel) and CBM (right upper panel) of (a) GeSe/$GeSnS_2$-Ge, (b) GeSe/$GeSnSe_2$-Ge, (c) GeSe/$GeSnSe_2$-Sn, (d) GeSe/Sn_2SSe-Se, (e) SnS/$GeSnS_2$-Ge and (f) SnSe/$GeSnSe_2$-Ge calculated from HSE06 functional. At the left panel, the blue and red plots indict the contribution from pristine and Janus monochalcogenides, respectively, and the width are proportional to the weight. The upper number is the CBO, and the lower number is the VBO. At the right panel, the isosurface of partial charge density is 0.004 e/$Born^3$.