Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information for

2D layered BP/InSe and BP/Janus In_2SeX (X=S or Te) type-II van der Waals heterostructures for photovoltaics: insight from first-principles calculations

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Table S1 Energy per layer in a unit cell of InSe, In_2SeTe and In_2SeS at different polymorphs.

	Energy (eV)		
	ε-	β-	γ-
InSe	−15.31(5)	−15.29(8)	−15.32(3)
In_2SeTe	−14.59(6)	−14.57(4)	−14.60(2)
In_2SeS	−15.88(2)	−15.86(9)	−15.88(8)

Table S2 Atomic and electronic structure information of BP, InSe, and Janus In_2SeX (X=S or Te) with bilayer (BL) and trilayer (TL): lattice constants (a, b), interlayer distance along the z direction (d), band gap (E_g), electron affinity (χ), and ionization energy (I) from PBE calculation and HSE06 calculation.

		a	b	d	E_g (eV)		χ (eV)		I (eV)	
		(Å)	(Å)	(Å)	PBE	HSE06	PBE	HSE06	PBE	HSE06
BL	BP	3.33	4.52	2.99	0.51	1.15	4.13	3.83	4.64	4.98
	InSe	4.05	7.01	2.95	1.02	1.72	4.64	4.44	5.66	6.16
	In_2SeTe(-Se)	4.18	7.25	2.99	0.78	1.57	4.81	4.47	5.59	6.04
	In_2SeTe(-Te)	4.18	7.25	2.99	0.78	1.57	4.30	4.04	5.08	5.61
	In_2SeS(-S)	3.96	6.86	2.93	1.14	1.95	4.95	4.65	6.09	6.60
	In_2SeS(-Se)	3.96	6.86	2.93	1.14	1.95	4.57	4.30	5.71	6.25
TL	BP	3.33	4.51	2.98	0.31	0.94	4.15	4.08	4.46	5.02
	InSe	4.05	7.01	2.95	0.79	1.48	4.74	4.53	5.53	6.01
	In_2SeTe(-Se)	4.18	7.25	2.99	0.51	1.08	4.99	4.90	5.50	5.98
	In_2SeTe(-Te)	4.18	7.25	2.99	0.51	1.08	4.33	4.09	4.84	5.17
	In_2SeS(-S)	3.96	6.86	2.93	0.89	1.67	5.11	4.85	6.00	6.52
	In_2SeS(-Se)	3.96	6.86	2.93	0.89	1.67	4.58	4.29	5.47	5.96

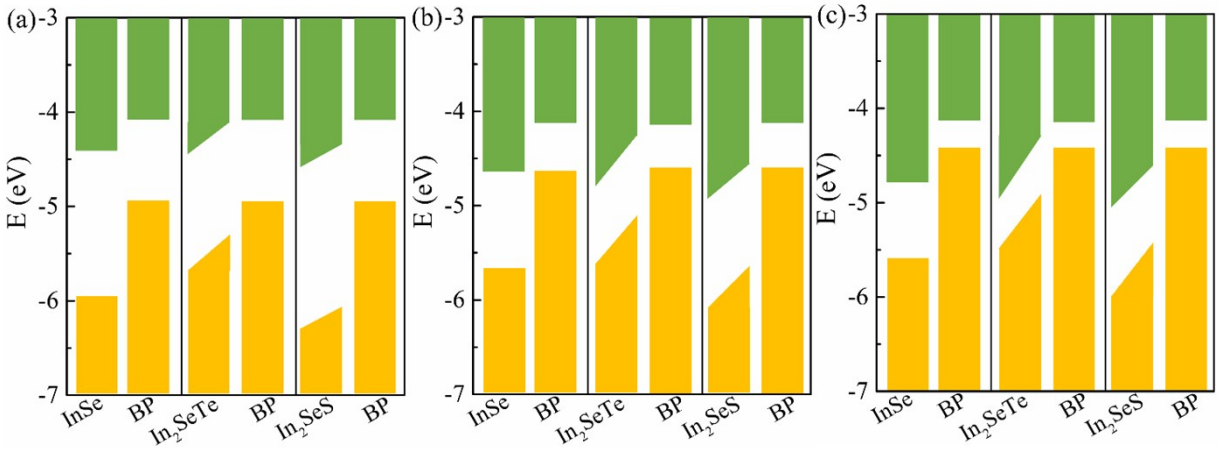

Fig. S1 Band alignments between BP and InSe, BP and In_2SeTe, as well as BP and In_2SeS of (a) monolayer, (b) bilayer, and (c) trilayer calculated with PBE functional.