Electronic Supplementary Material for

InSe/Te van der Waals Heterostructure as a High-Efficiency Solar Cell from Computational Screening

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Table S1. The lattice constants a (Å), the M-M, M-X_A and X_B-X_B (M = Al, Ga, In, X_A = S, Se, Te and X_B = Se, Te) bond lengths $L_{M\text{-}M}$ (Å), $L_{M\text{-}X_A}$ (Å) and $L_{X_B\text{-}X_B}$ (Å), the PBE and HSE band gaps E_g^{PBE} (eV), E_g^{HSE} (eV) for the MX_A and X_B monolayers

System	a	$L_{M\text{-}M}$	$L_{M\text{-}X_A}$	$L_{X_B\text{-}X_B}$	E_g^{PBE}	E_g^{HSE}
AlS	3.563	2.588	2.320		2.19	3.16
AlSe	3.776	2.586	2.472		1.97	2.97
AlTe	4.116	2.573	2.700		1.88	2.71
GaS	3.612	2.466	2.362		2.41	3.46
GaSe	3.787	2.462	2.492		1.85	2.82
GaTe	4.096	2.459	2.696		1.48	2.22
InS	3.893	2.800	2.556		1.76	2.66
InSe	4.041	2.797	2.677		1.51	2.32
InTe	4.327	2.790	2.875		1.43	2.16
Se	3.714			2.668	0.61	1.14
Te	4.185			3.036	0.59	1.09

Table S2. The energy differences ΔE (meV) and interlayer distances d (Å) as well as the lattice constants a (Å) and bond lengths L (Å) of various configurations for AlX_A/X_B vdW heterostructures

System	Configuration	ΔE	d	a	$L_{M\text{-}M}$	$L_{M\text{-}X_A}$	$L_{X_A\text{-}X_B}$
AlS-Se	a	3	3.159	3.627	2.587	2.339	2.649
	b	5	3.138	3.629	2.587	2.340	2.652
	c	61	3.608	3.625	2.588	2.339	2.648
	d	0	3.123	3.627	2.588	2.340	2.651
	e	62	3.617	3.624	2.587	2.337	2.647
	f	6	3.160	3.629	2.586	2.340	2.652
AlS-Te	a	1	3.273	3.821	2.578	2.401	2.984
	b	14	3.264	3.826	2.580	2.404	2.984
	c	66	3.728	3.817	2.577	2.399	2.982
	d	0	3.617	3.822	2.579	2.402	2.985
	e	69	3.389	3.817	2.578	2.399	2.982
	f	12	3.273	3.826	2.580	2.403	2.984
AlSe-Se	a	4	3.156	3.741	2.579	2.462	2.674
	b	2	3.070	3.744	2.580	2.462	2.678
	c	72	3.652	3.736	2.580	2.460	2.672
	d	0	3.089	3.744	2.580	2.462	2.678
	e	73	3.663	3.737	2.580	2.460	2.671
	f	4	3.124	3.744	2.579	2.462	2.678
AlSe-Te	a	3	3.272	3.934	2.576	2.522	2.997
	b	11	3.184	3.939	2.574	2.522	2.999
	c	75	3.815	3.932	2.574	2.520	3.000
	d	0	3.180	3.935	2.573	2.522	2.999
	e	78	3.822	3.930	2.575	2.520	2.996
	f	11	3.271	3.938	2.573	2.522	2.995
AlTe-Se	a	21	3.075	3.953	2.567	2.656	2.721
	b	0	2.908	3.965	2.568	2.659	2.736
	c	122	3.763	3.943	2.567	2.654	2.730
	d	16	3.042	3.956	2.566	2.655	2.732
	e	122	3.754	3.943	2.567	2.653	2.720
	f	10	3.033	3.956	2.568	2.657	2.718
AlTe-Te	a	7	3.307	4.126	2.566	2.705	3.027
	b	7	3.220	4.136	2.566	2.707	3.033
	c	100	3.951	4.121	2.565	2.702	3.030
	d	0	3.212	4.129	2.566	2.704	3.031
	e	101	3.965	4.119	2.566	2.701	3.023
	f	12	3.285	4.131	2.565	2.706	3.023

Table S3. The energy differences ΔE (meV) and interlayer distances d (Å) as well as the lattice constants a (Å) and bond lengths L (Å) of various configurations for GaX_A/X_B vdW heterostructures

System	Configuration	ΔE	d	a	$L_{M\text{-}M}$	$L_{M\text{-}X_A}$	$L_{X_A\text{-}X_B}$
GaS-Se	a	6	3.104	3.656	2.466	2.375	2.656
	b	5	3.037	3.660	2.467	2.376	2.653
	c	71	3.585	3.654	2.468	2.374	2.654
	d	0	3.020	3.660	2.468	2.377	2.657
	e	72	3.598	3.654	2.468	2.375	2.659
	f	8	3.092	3.659	2.467	2.376	2.657
GaS-Te	a	7	3.153	3.861	2.477	2.442	2.987
	b	14	3.081	3.866	2.477	2.443	2.987
	c	78	3.647	3.855	2.478	2.438	2.991
	d	0	3.062	3.863	2.476	2.443	2.991
	e	80	3.671	3.856	2.476	2.439	2.994
	f	18	3.158	3.865	2.476	2.442	2.989
GaSe-Se	a	5	3.068	3.765	2.464	2.487	2.683
	b	0.1	2.969	3.770	2.465	2.488	2.677
	c	81	3.658	3.757	2.463	2.484	2.676
	d	0	3.020	3.764	2.463	2.487	2.679
	e	82	3.647	3.758	2.462	2.485	2.683
	f	5	3.059	3.765	2.463	2.488	2.677
GaSe-Te	a	8	3.169	3.959	2.474	2.548	3.001
	b	11	3.081	3.967	2.472	2.549	3.003
	c	92	3.747	3.954	2.470	2.544	3.003
	d	0	3.083	3.963	2.472	2.548	3.004
	e	93	3.732	3.954	2.471	2.544	2.999
	f	18	3.160	3.965	2.473	2.548	3.003
GaTe-Se	a	27	3.004	3.965	2.457	2.663	2.735
	b	0	2.833	3.980	2.456	2.665	2.723
	c	140	3.722	3.950	2.452	2.660	2.722
	d	22	2.963	3.970	2.455	2.662	2.726
	e	140	3.733	3.955	2.455	2.659	2.735
	f	13	2.911	3.969	2.456	2.665	2.736
GaTe-Te	a	8	3.208	4.134	2.464	2.713	3.027
	b	4	3.113	4.149	2.464	2.714	3.037
	c	113	3.915	4.129	2.461	2.707	3.031
	d	0	3.126	4.141	2.464	2.712	3.036
	e	113	3.954	4.130	2.462	2.708	3.024
	f	15	3.209	4.141	2.463	2.713	3.033

Table S4. The energy differences ΔE (meV) and interlayer distances d (Å) as well as the lattice constants a (Å) and bond lengths L (Å) of various configurations for InX_A/X_B vdW heterostructures

System	Configuration	ΔE	d	a	$L_{M\text{-}M}$	$L_{M\text{-}X_A}$	$L_{X_A\text{-}X_B}$
InS-Se	a	8	2.963	3.823	2.799	2.543	2.695
	b	0	2.862	3.829	2.798	2.544	2.692
	c	89	3.562	3.814	2.798	2.541	2.691
	d	1	2.876	3.825	2.799	2.544	2.694
	e	90	3.562	3.816	2.800	2.541	2.697
	f	6	2.947	3.824	2.798	2.543	2.696
InS-Te	a	10	3.054	4.023	2.811	2.593	3.010
	b	5	2.961	4.029	2.810	2.595	3.011
	c	95	3.632	4.018	2.811	2.591	3.013
	d	0	2.964	4.024	2.811	2.593	3.012
	e	97	3.643	4.018	2.811	2.591	3.013
	f	14	3.005	4.029	2.813	2.594	3.012
InSe-Se	a	14	2.918	3.913	2.793	2.653	2.720
	b	0	2.776	3.921	2.795	2.655	2.713
	c	108	3.581	3.903	2.791	2.649	2.712
	d	8	2.840	3.915	2.793	2.652	2.715
	e	108	3.567	3.903	2.793	2.650	2.719
	f	8	2.864	3.914	2.794	2.653	2.719
InSe-Te	a	10	3.041	4.108	2.806	2.699	3.025
	b	3	2.931	4.117	2.805	2.700	3.027
	c	105	3.690	4.102	2.804	2.696	3.023
	d	0	2.980	4.112	2.804	2.700	3.027
	e	106	3.730	4.103	2.800	2.696	3.022
	f	13	3.036	4.112	2.804	2.700	3.024
InTe-Se	a	55	2.844	4.095	2.780	2.833	2.770
	b	0	2.521	4.124	2.782	2.842	2.754
	c	187	3.683	4.075	2.778	2.827	2.763
	d	49	2.768	4.105	2.780	2.832	2.758
	e	187	3.672	4.077	2.779	2.828	2.764
	f	23	2.662	4.106	2.782	2.843	2.773
InTe-Te	a	14	3.103	4.272	2.790	2.869	3.059
	b	0	2.932	4.290	2.792	2.872	3.064
	c	133	3.891	4.264	2.787	2.863	3.057
	d	6	3.027	4.281	2.789	2.869	3.062
	e	133	3.893	4.266	2.790	2.864	3.050
	f	12	3.061	4.278	2.790	2.871	3.059

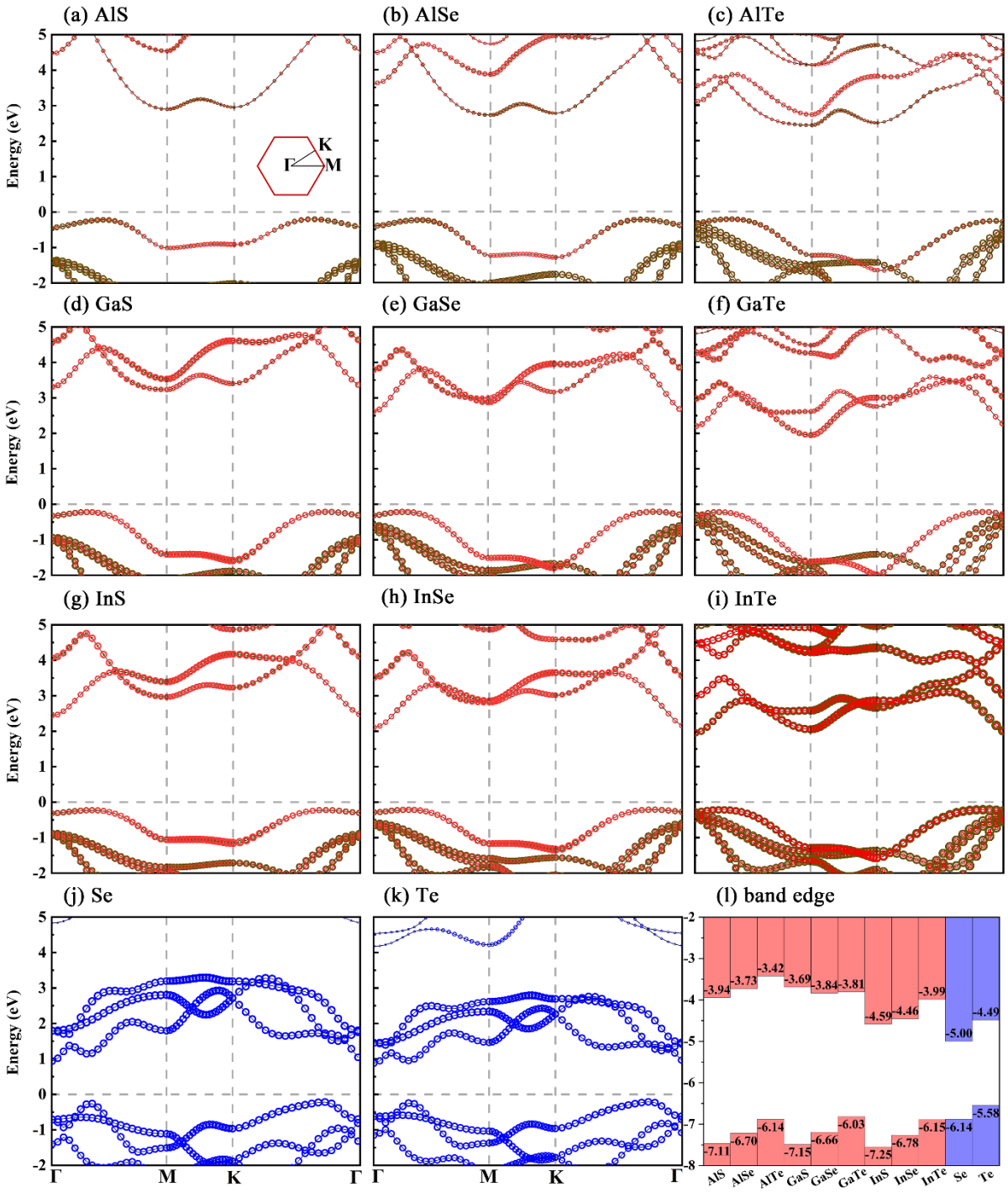

Figure S1. Projected band structures of (a) AlS, (b) AlSe, (c) AlTe, (d) GaS, (e) GaSe, (f) GaTe, (g) InS, (h) InSe, (i) InTe, (j) Se and (k) Te monolayers by HSE06 hybrid functional method. The red, brown, blue circles represent the projected specific gravity of M, X_A, X_B atoms, respectively. The first Brillouin zone with high-symmetry points are shown in the inset of (a). (l) The band edge alignments of these monolayers.