Supporting Information

Type-II Lateral SnSe/GeTe Heterostructure for Solar Photovoltaic Applications with High Efficiency

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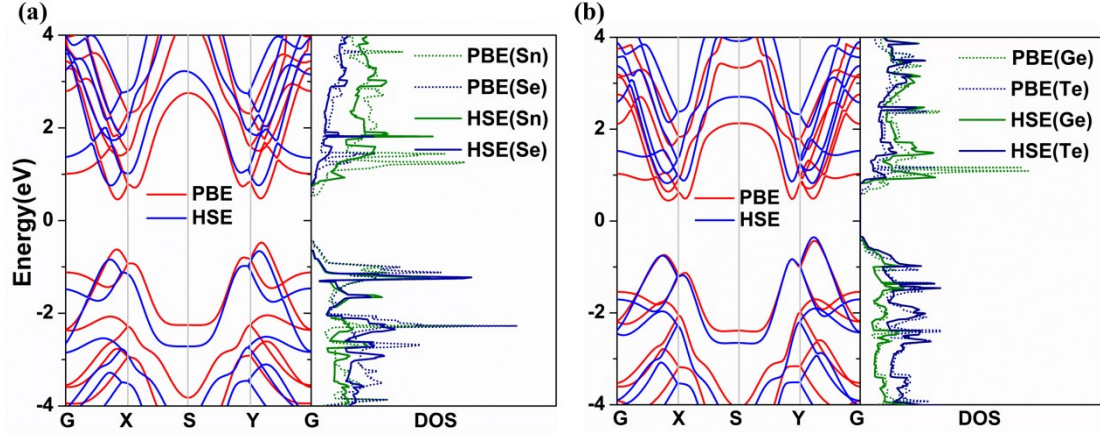
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Fig. S1 The band structure and projected density of states for monolayer (a) SnSe (b) GeTe.

Table S1 Equilibrium 2D Lattice Parameters and bandgaps calculated by PBE and HSE06 methods.

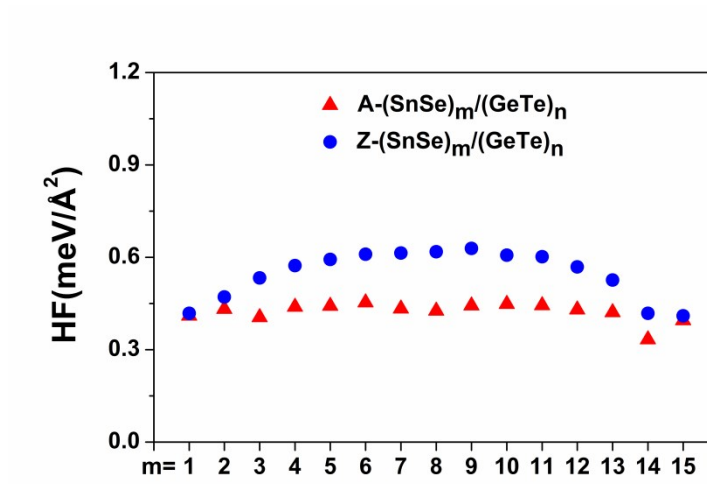|	This work				Ref.[9]			
	a(Å)	b(Å)	$E_{g\text{-PBE}}$(eV)	$E_{g\text{-HSE}}$(eV)	a(Å)	b(Å)	$E_{g\text{-PBE}}$(eV)	$E_{g\text{-HSE}}$(eV)
SnSe	4.29	4.39	0.93	1.41	4.28	4.43	1.00	1.44
GeTe	4.24	4.37	0.88	1.17	4.23	4.47	0.95	1.24

Fig. S2 Heat of formation (HF) of heterostructures with $m + n = 16$. The red triangle represents A-(SnSe)$_m$/(GeTe)$_n$ and blue circle represents Z-(SnSe)$_m$/(GeTe)$_n$.
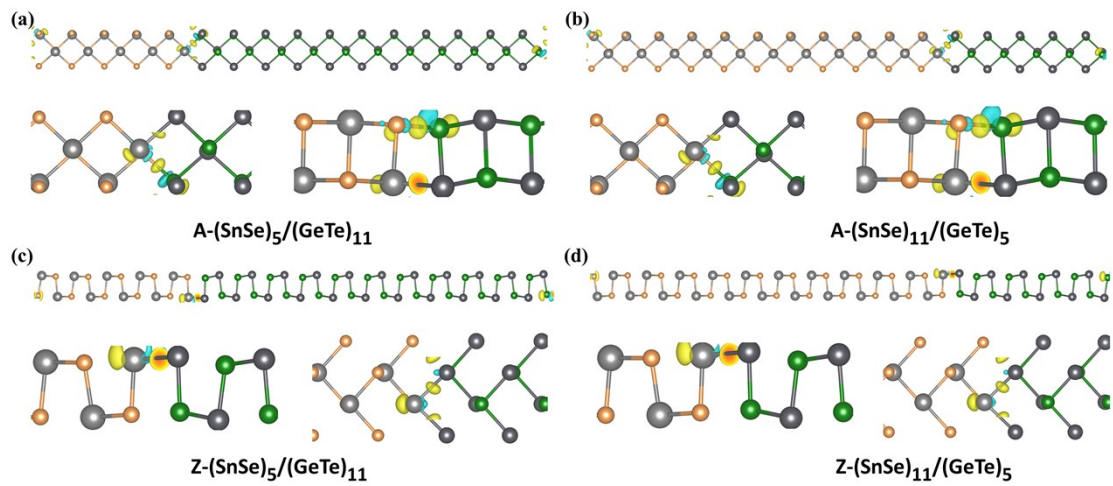
Fig. S3 The electron density difference of (a) A-$(SnSe)_5$/$(GeTe)_{11}$, (b) A-$(SnSe)_{11}$/$(GeTe)_5$, (c) Z-$(SnSe)_5$/$(GeTe)_{11}$ and (d) Z-$(SnSe)_{11}$/$(GeTe)_5$. The left and right sides are the side view and top view near the interface, respectively.
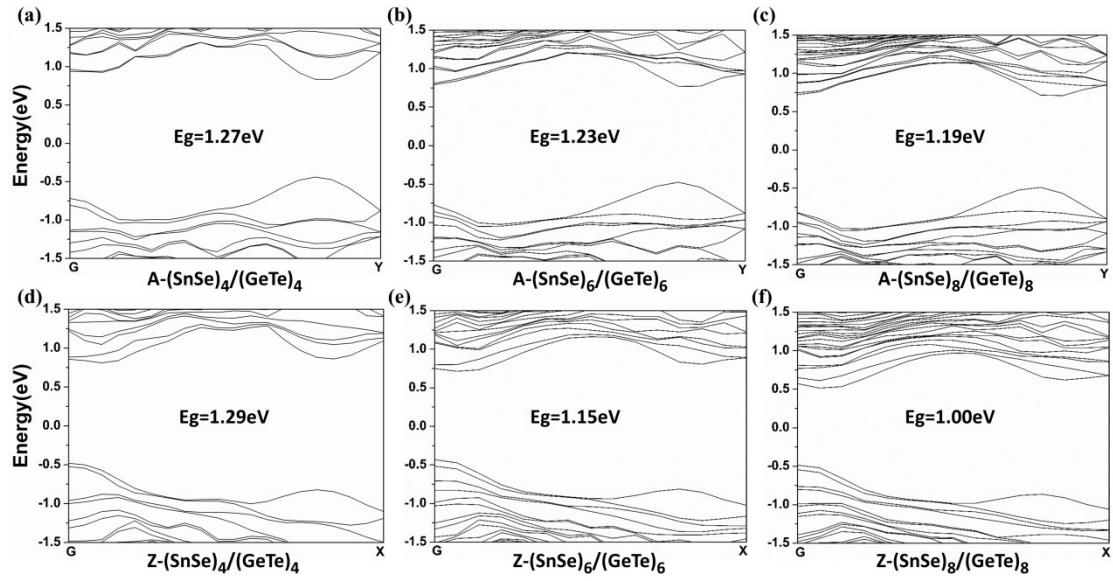
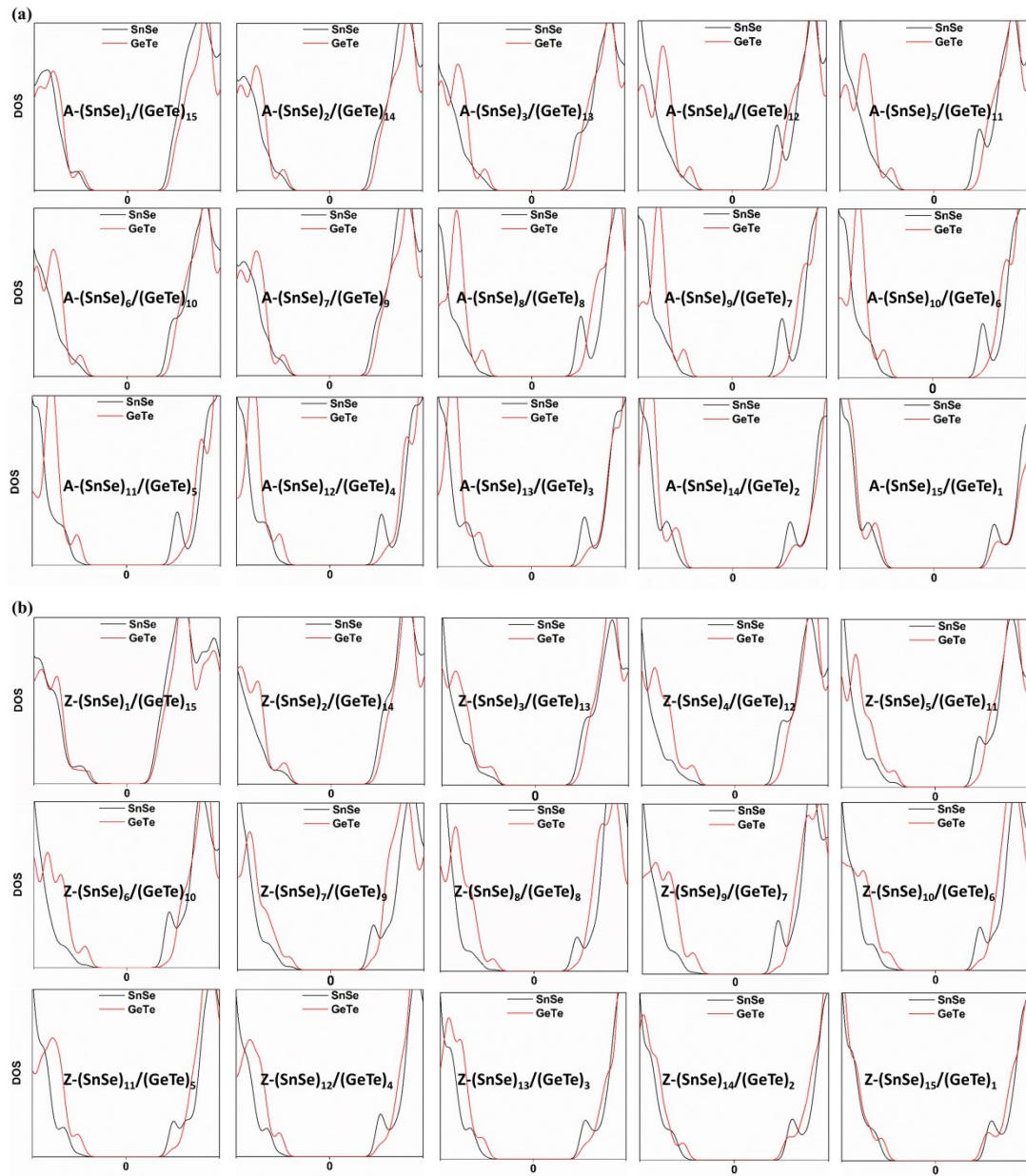**Fig. S4** Band structures of heterostructures with m(n)=4~8 obtained by HSE06 method.

Fig. S5. The local density of states in the center of (a) A-$(SnSe)_m$/$(GeTe)_n$ and (b) Z-$(SnSe)_m$/$(GeTe)_n$.

Table S2 The J_{abs} and PCE values of $(SnSe)_m/(GeTe)_n$.

SnSe/GeTe (m/n)	Jabs (mA/cm^2)		PCE (%)	
	armchair	zigzag	armchair	zigzag
1/15	5.12	4.84	21.22	21.27
2/14	5.10	4.75	20.58	20.53
3/13	5.04	4.51	20.57	21.20
4/12	4.97	4.61	20.54	20.22
5/11	4.79	4.54	20.56	19.41
6/10	4.83	4.47	20.57	19.80
7/9	4.63	4.40	20.81	19.85
8/8	4.55	4.19	20.85	20.14
9/7	4.52	4.26	20.85	19.96
10/6	4.46	4.13	21.17	20.95
11/5	4.33	4.04	21.17	21.30
12/4	4.21	3.93	21.22	21.48
13/3	4.10	3.84	21.12	21.56
14/2	3.98	3.54	21.38	type I
15/1	3.85	3.56	21.41	type I