Supporting information

First-Principles Study of Interface Properties of $CsSnI_3$-SnS heterostructure

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Table S1 Bandgaps (HSE06 functional) of SnS monolayer, CsI interface and SnI_2 interface at pre-contact state and contact state in the $CsSnI_3$-SnS heterostructure.

	SnS-CsI		SnS-SnI_2	
	SnS	CsI	SnS	SnI_2
Pre-contact	2.08	1.48	2.18	1.68
Contact	1.92	1.46	2.39	1.28

Table S2 Comparison between the calculated and experimental values of the bandgap of $CsSnI_3$ and SnS

	calculated value		experiment value	Other calculated values
	PBE	HSE06		
$CsSnI_3$	0.83	1.28	1.3[1]	1.04[3]
SnS	0.98	1.19	1.3[2]	1.07[4]

References

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Fig. S1 The molecular dynamics simulation is calculated for the (a) CsI/SnS and (b) SnI_2/SnS heterostructures at room temperature (300K).

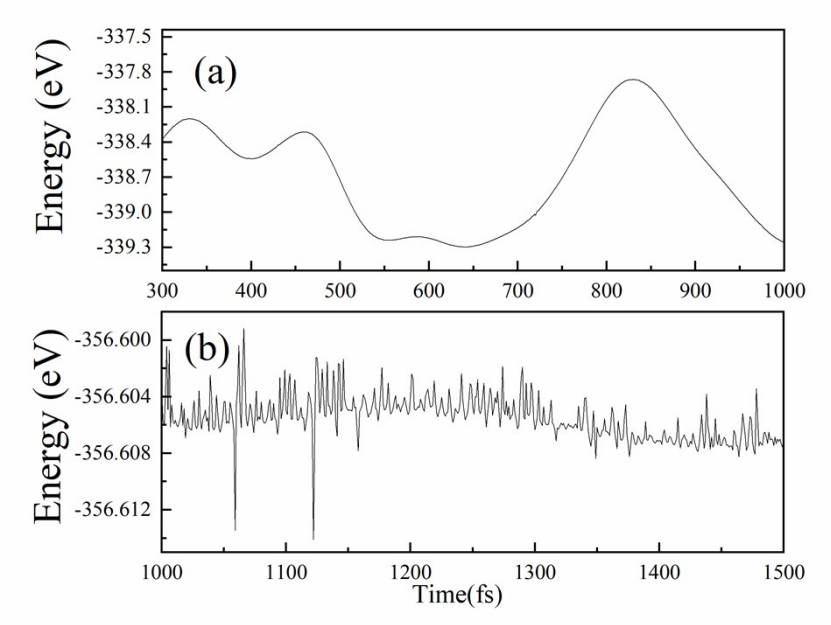

Fig. S2 Band structures of (a) CsI-SnS and(b) SnI_2-SnS heterostructure. The blue and red lines denote the contribution from $CsSnI_3$ and SnS, respectively. The Fermi level is set at zero.

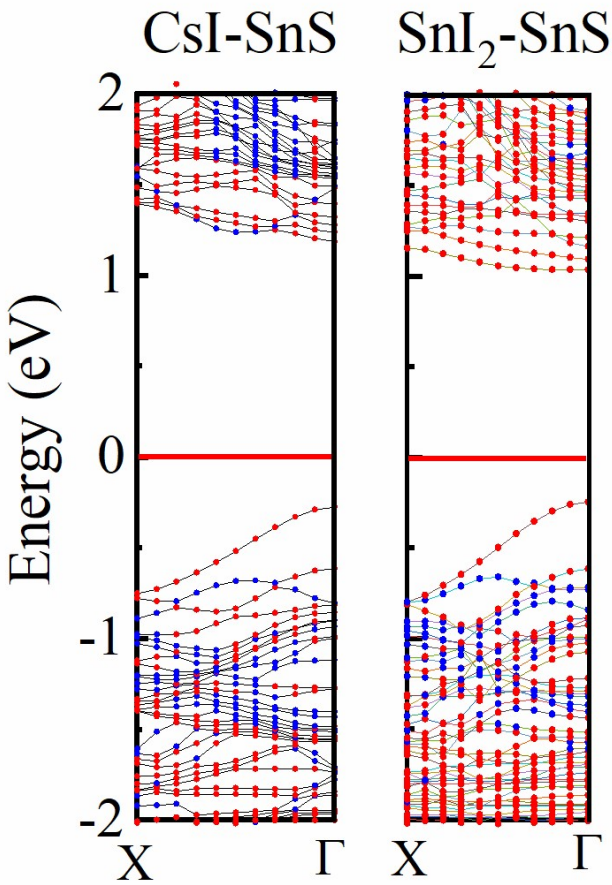
CsI-SnS
SnI2-SnS
Energy (eV)
2
1
0
-1
-2
X
Γ
X
Γ

Fig. S3 The total density of states (DOS) of I, Sn , Cs, and S atoms of (a) CsI-SnS and (b) SnI_2-SnS heterostructure. The DOS of interfacial atomic states of Sn and I in (c) CsI-SnS interface and Sn and S atom in SnI_2-SnS interface.