Supplemental Material

High-performance and self-powered photodetectors from S-scheme $Cs_2SnI_2Cl_2/Cs_2TiI_6$ heterojunction: A DFT+NAMD study

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Table 1S Band gaps of Cs_2TiI_6 and $Cs_2SnI_2CI_2$ obtained by different methods

System	GGA-PBE	HSE06	HSE06+SOC	$GGA\_1/2$	Experiment
Cs_2TiI_6	0.86 eV	1.90 eV	1.7 eV [1]	1.03 eV	1.02 eV [2]
$Cs_2SnI_2CI_2$	1.59 eV	2.23 eV	2.07 eV [3]	2.34 eV	2.62 eV [4]

Table 2S Calculated effective masses of electrons and holes for $Cs_2SnI_2CI_2$ surface，Cs_2TiI_6 surface and $Cs_2SnI_2CI_2/Cs_2TiI_6$ heterojunction

	m_h^*/m_0	m_e^*/m_0	m_h^*/m_0	m_e^*/m_0
	Γ → X		Γ → M	
$Cs_2SnI_2Cl_2/Cs_2TiI_6$	0.63	0.35	0.64	0.34
$Cs_2SnI_2Cl_2$	1.03	0.40	1.05	1.43
	M → X	Γ → X	M → Γ	Γ → M
Cs_2TiI_6	0.02	0.31	0.01	0.31

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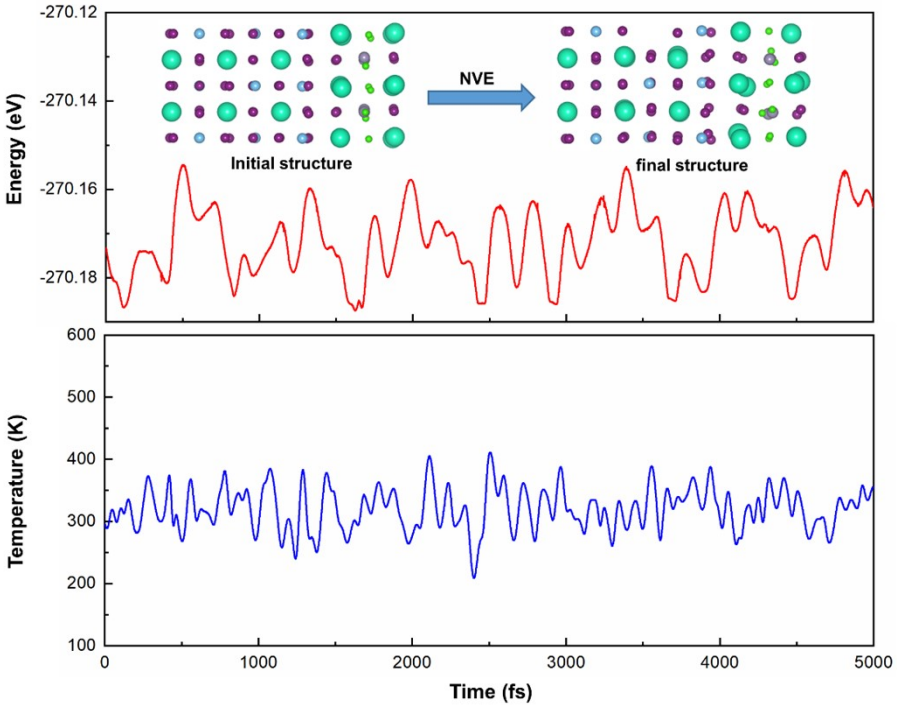

Fig. 1S Total energy and temperature fluctuations with respect to molecular dynamic steps at 300K for $Cs_2SnI_2CI_2/Cs_2TiI_6$ heterojunction

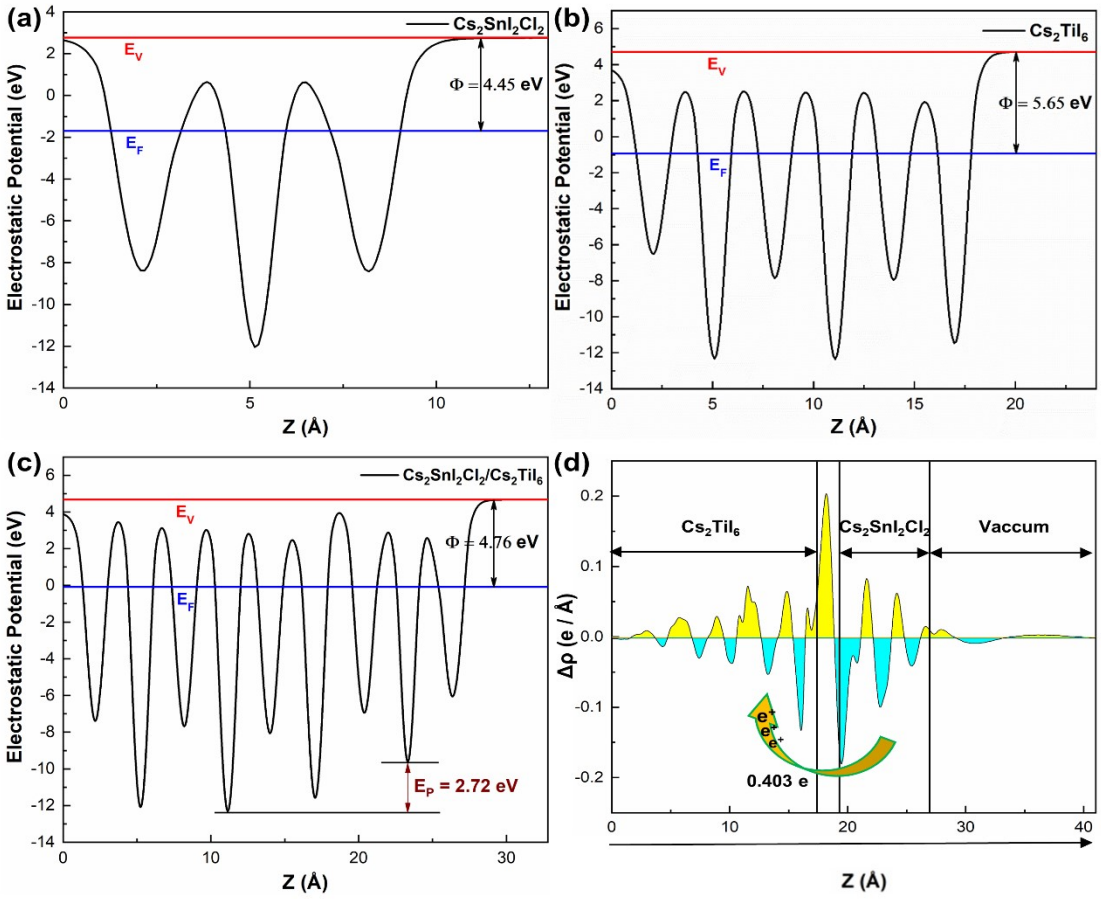

Fig. 2S The work functions of (a) $Cs_2SnI_2CI_2$ surface, (b) Cs_2TiI_6 surface and (c)

$Cs_2SnI_2CI_2/Cs_2TiI_6$. E_v, E_f and E_p are vacuum level, fermi level and interface potential drop, respectively. (d) The planar-averaged charge density difference $\Delta\rho$ for $Cs_2SnI_2CI_2/Cs_2TiI_6$ heterojunction. The cyan and yellow sections show electron depletion and concentration, respectively.

References

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