Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Insight into electron transport performance of $FAPbI_3/SnO_2$ interface

Xiangxiang Feng [1], Biao Liu [1*], Mengqiu Cai [2], Junliang Yang [1]

1. Hunan Key Laboratory for Super-microstructure and Ultrafast Process, School of Physics and Electronics, Central South University, Changsha 410083, Hunan, China

2. School of Physics and Electronics Science, Hunan University, Changsha 410082, Hunan, China

*Corresponding author. E-mail: bliu612@csu.edu.cn.

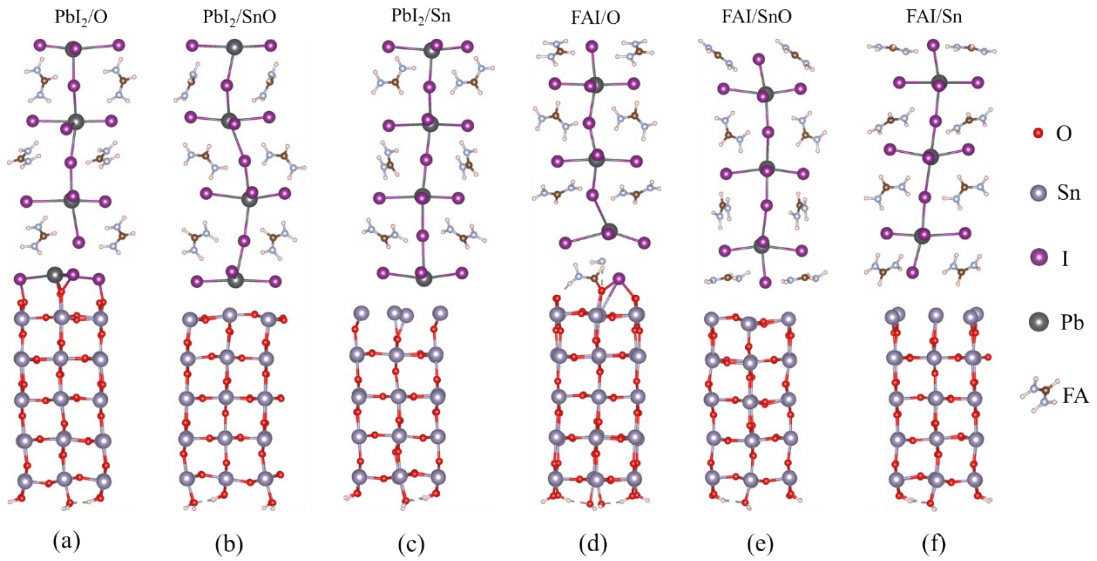

FIG. S1. Representative snapshot of AIMD trajectory at 300 K. (a-c) The PbI_2/O, PbI_2/SnO and PbI_2/Sn interfaces. (d-f) The FAI/O, FAI/SnO and FAI/Sn interfaces.

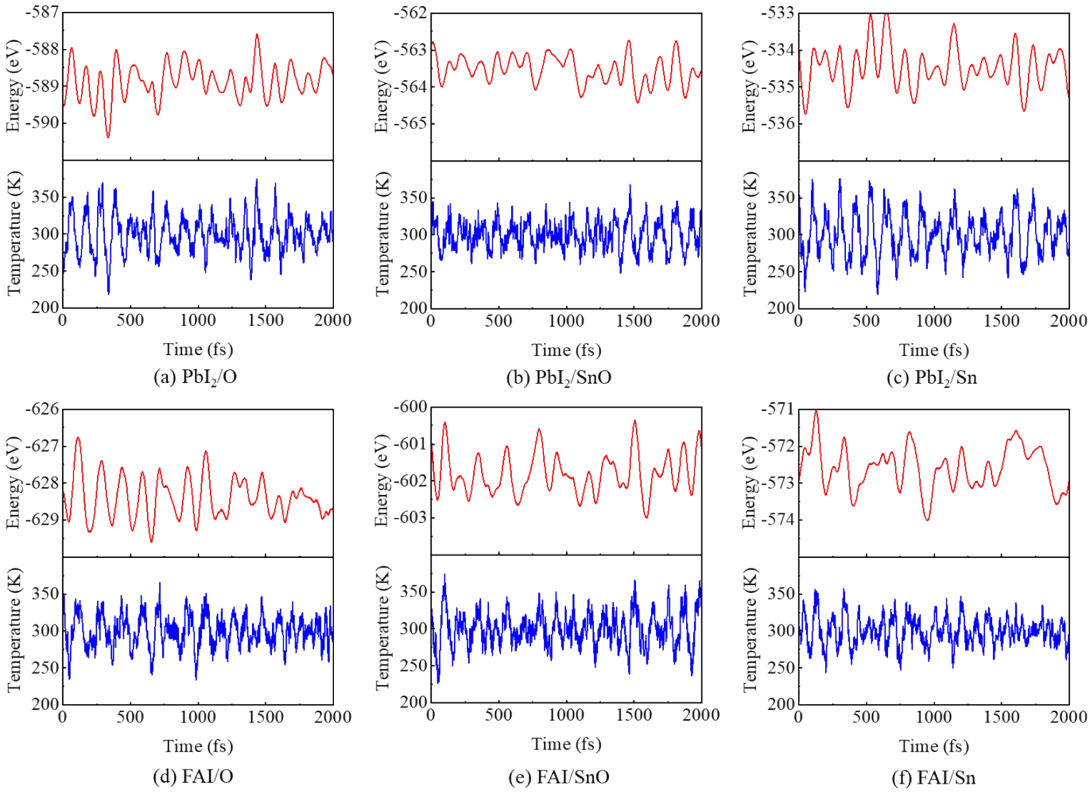

FIG. S2. AIMD simulations of the interfaces at the 300K. Red lines represent fluctuations of energy with time, and blue lines represent fluctuations of temperature with time. (a-c) The PbI_2/O, PbI_2/SnO and PbI_2/Sn interfaces. (d-f) The FAI/O, FAI/SnO and FAI/Sn interfaces.

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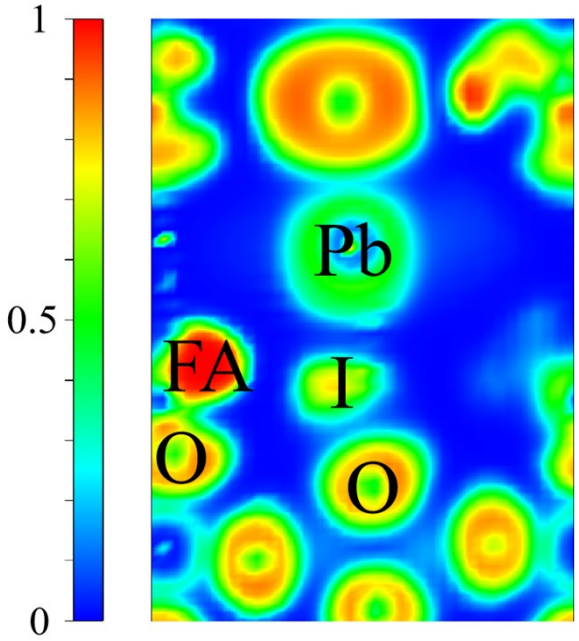

FIG. S3. 2D maps of the ELF fields perpendicular to the FAI/O interface. One means complete electron localization, and zero means complete electron delocalization.

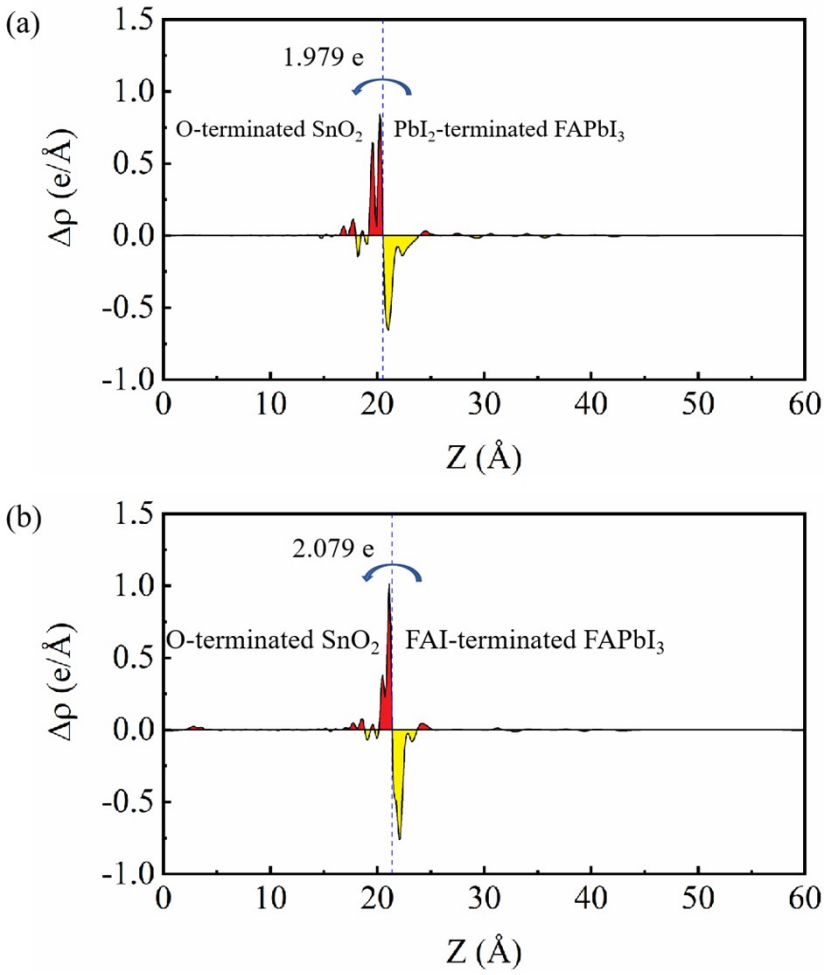

FIG. S4. Plane-averaged charge density difference along the Z direction coupling with Bader charge analysis in the (a) PbI_2/O interface and (b) FAI/O interface.

*The charge density difference Δρ is given by:

$$\Delta\rho = \rho_{A+B} - \rho_A - \rho_B \quad (1)$$

Where ρ_{A+B}, ρ_A and ρ_B are the plane-averaged charge density of the total heterostructures, free-standing A slab, and free-standing B slab, respectively.

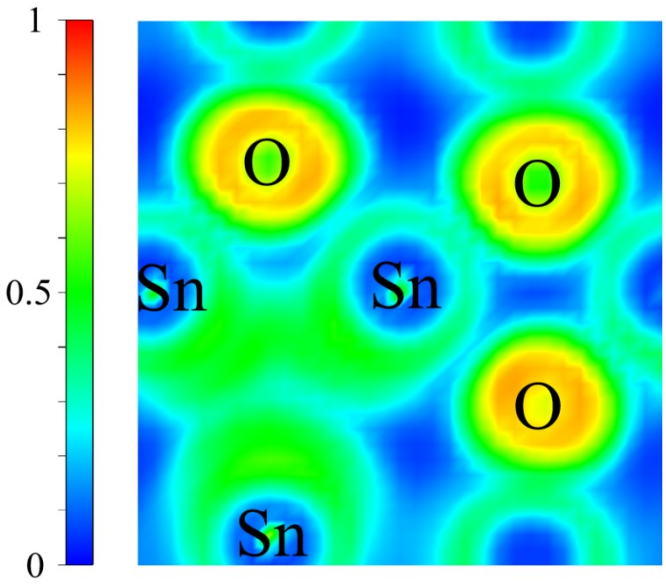

FIG. S5. 2D map of the ELF field on the SnO surface of PbI_2/SnO interface with an O vacancy. One means complete electron localization, and zero means complete electron delocalization.

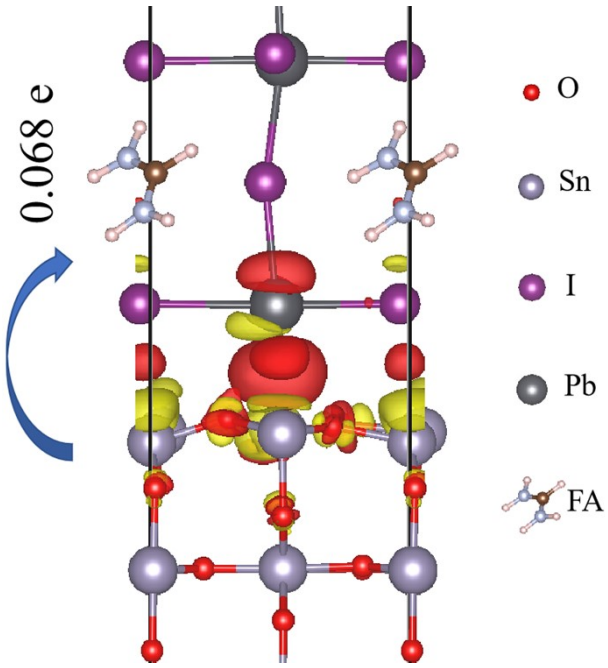

FIG. S6. Charge density difference coupling with Bader charge analysis on the PbI_2/SnO interface with an O vacancy. The value of the isosurface is 1×10^{-3} e per born^3. Red represents gain electrons, and yellow represents lose electrons.

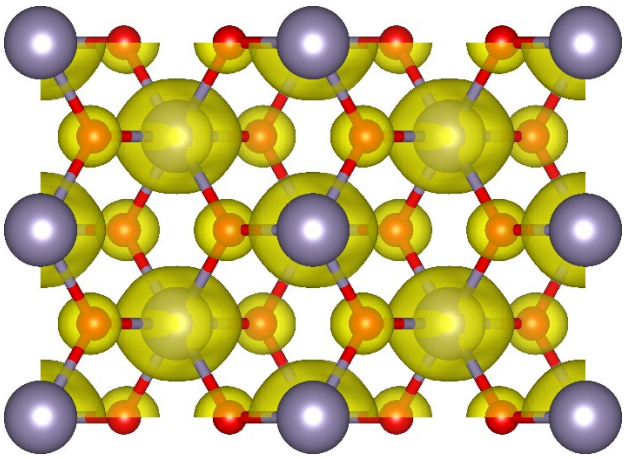

FIG. S7. Charge density at SnO_2 conduction band minimum.

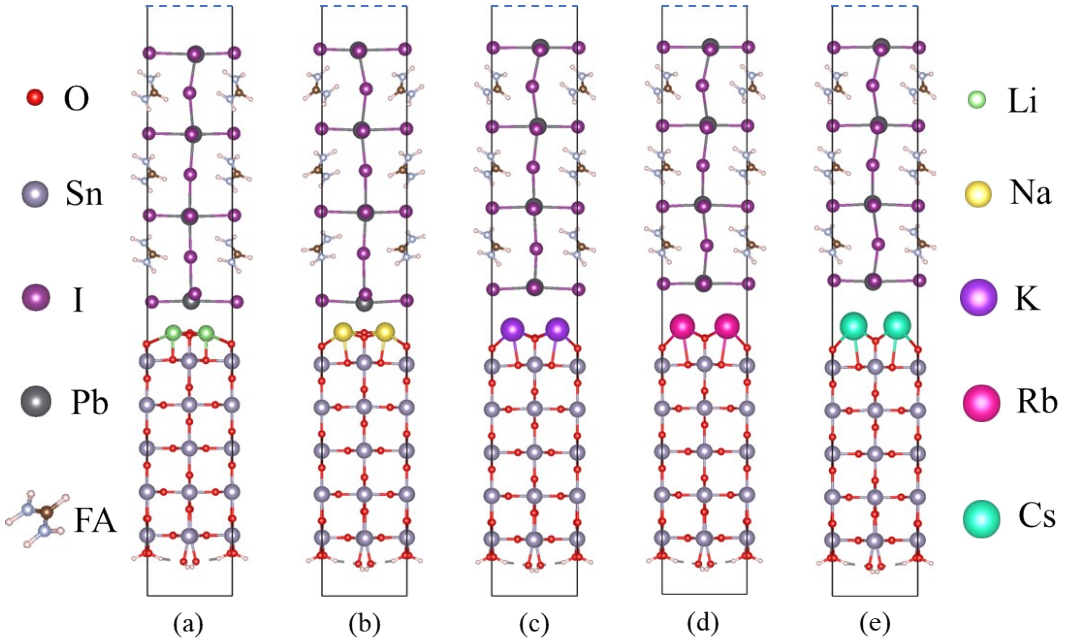

FIG. S8. Side views of the PbI_2/O interfaces modified by the alkali metal elements [(a) Li, (b) Na, (c) K, (d) Rb and (e) Cs].

Table SI. Calculated lattice parameters (in Å) of $FAPbI_3$, SnO_2 and SnI_4 bulk.

		$FAPbI_3$	SnO_2	SnI_4
This work	x	6.415	4.832	6.757
	y	6.415	4.832	6.757
	z	6.415	3.243	6.757
Other work	x	6.352[1]	4.737[2]	6.686[3]
	y	6.352	4.737	6.686
	z	6.352	3.185	6.686

Table SII. The relaxed lattice parameters (in Å) for the $FAPbI_3/SnO_2$ interface models.

	PbI_2/O,	PbI_2/SnO	PbI_2/Sn	FAI/O	FAI/SnO	FAI/Sn
x	6.39	6.43	6.42	6.38	6.39	6.40
y	6.68	6.68	6.64	6.66	6.69	6.64
z			60			

Table SIII. Interface binding energies (in meV/Å^2) of $FAPbI_3/SnO_2$ interface.

$FAPbI_3$-SnO_2	PbI_2	FAI
O	-65.8	-70.5
SnO	-4.7	-4.2
Sn	-16.4	-14.4

*The interface binding energies ΔE is given by:

$$\Delta E = \frac{E_{A+B} - E_A - E_B}{S} \quad (2)$$

Where S is the area of the interface, E_A is the energy of A slab, E_B is the energy of B slab and E_{A+B} is the total energy of the heterostructure in the heterostructure lattice.

(1) Slimi, B.; Mollar, M.; Assaker, I. B.; Kriaa, I.; Chtourou, R.; Marí, B. *Energy Procedia.* **2016,** *102*, 87-95.

(2) Dhage, S.; Samuel, V.; Pasricha, R.; Ravi, V. *Ceram. Int.* **2006,** *32* (8), 939-941.

(3) Dawson, M.; Ribeiro, C.; Morelli, M. R. *Mater. Sci. Semicond. Process.* **2021,** *132*, 105908.