Supporting information

A first-principle study of the stability, electronic structure, and optical properties of halide double perovskite $Rb_2Sn_{1-x}Te_xI_6$ for solar cell applications

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1. Mechanical Properties

For mechanical properties, the elastic constants are calculated using the well-known stress–strain relationship (Hooke's law)[1] by deforming the unit cell. The elastic tensor C_{ij} can be calculated as

$$\delta_{ij} = C_{ij}.\varepsilon_{ij} \quad (1)$$

where δ_{ij} and ε_{ij} are stress and strain tensors. For cubic symmetry, only three independent components (C_{11}, C_{12}, and C_{44}) are needed. To check the mechanical stability for cubic compounds, the elastic constant must satisfy the generalized Born stability conditions[2]:

$$1/3(C_{11}+2C_{12})>0,\ C_{11}>0,\ C_{44}>0,\ \text{and}\ 1/2(C_{11}-C_{12})>0 \quad (2)$$

In addition to this, the Voigt-Reuss-Hill model[3-4] can be used to determine the other elastic parameters, such as bulk modulus (B), shear modulus (G), Young's modulus (E), Pugh's index ($k = B/G$), anisotropy factor (A), and Passion's ratio (**v**) using standard relations. The calculated elastic constants of the pure and doped system are enlisted in Table S5. It is evident that all the system satisfy the Born stability criteria, thus showing the mechanical stability. The Cauchy pressure (C_{11}-C_{44}) gives information about the ductility and brittleness of a compound. The positive (negative) value of C_{11}–C_{44} indicates the ductile (brittle) nature. From Table S5, it is inferred that the computed values of C_{11}–C_{44} are positive, implying the ductile nature for all these systems.

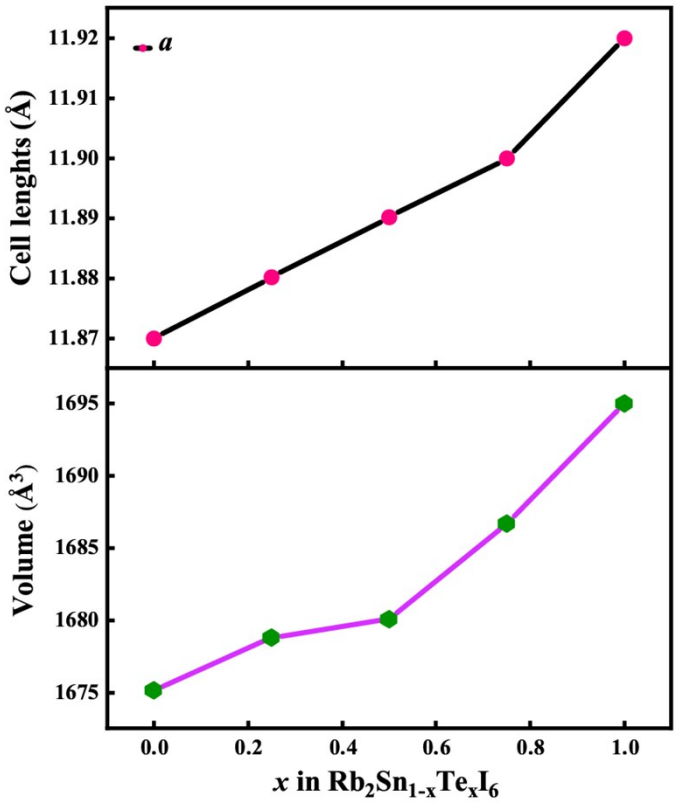

Fig. S1. The lattice parameter (top) and volume (bottom) as a function of ***x*** in $Rb_2Sn_{1-x}Te_xI_6$ ($0 \leq x \leq 1$).

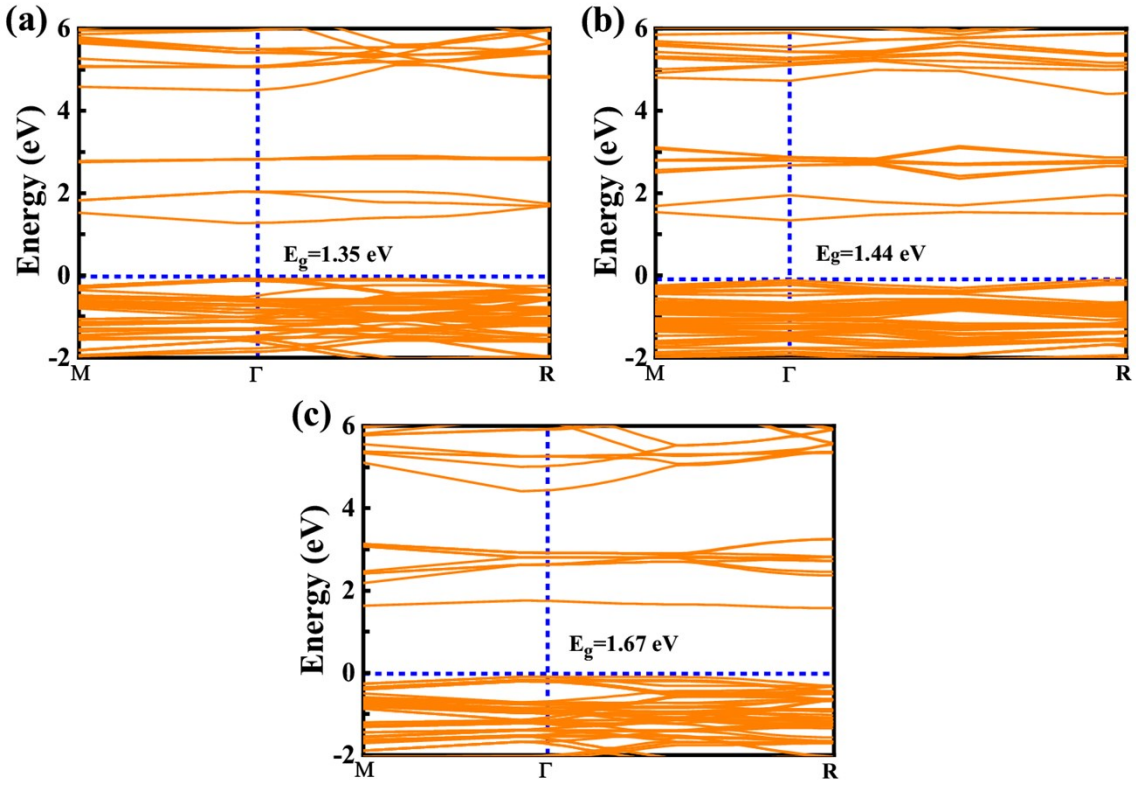

Fig. S2. Calculated band structure of $Rb_2Sn_{0.75}Te_{0.25}I_6$ (a), $Rb_2Sn_{0.50}Te_{0.50}I_6$ (b), and $Rb_2Sn_{0.25}Te_{0.75}I_6$ (c) using HSE06 functional.

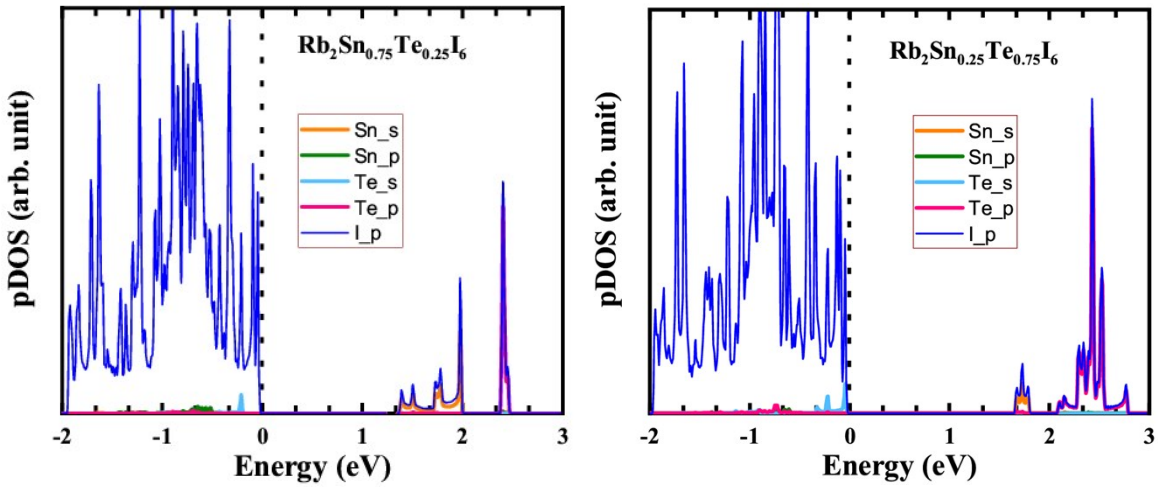

Fig. S3. DOS structures of $Rb_2Sn_{0.75}Te_{0.25}I_6$ (left) and $Rb_2Sn_{0.25}Te_{0.75}I_6$ (right) using HSE06 functional.

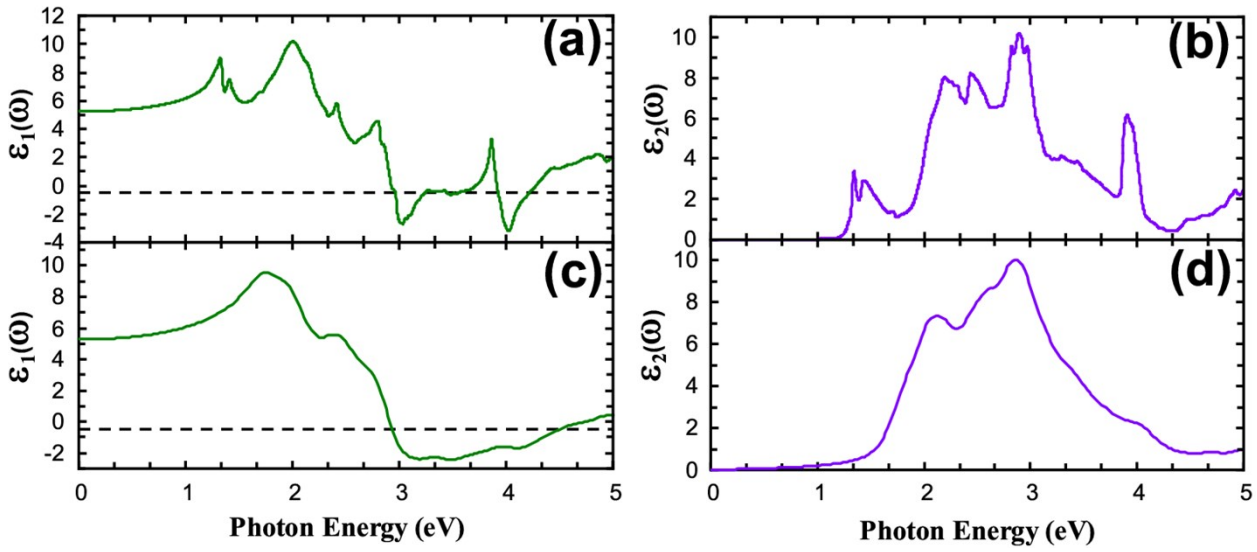

Fig. S4. (a, c) Calculated real $\varepsilon_1(\omega)$ and (b, d) imaginary $\varepsilon_2(\omega)$ parts of the dielectric function of $Rb_2Sn_{0.25}Te_{0.75}I_6$ and Rb_2TeI_6 perovskites.

Table S1. Calculated bond lengths and angles for $Rb_2Sn_{1-x}Te_xI_6$ ($0 \leq x \leq 1$) alloyed systems.

Sort	Rb_2SnI_6	$Rb_2Sn_{0.75}Te_{0.25}I_6$	$Rb_2Sn_{0.50}Te_{0.50}I_6$	$Rb_2Sn_{0.25}Te_{0.75}I_6$	Rb_2TeI_6
Rb-(Sn/Te)/ Å	5.13	5.14/5.14	5.14/5.15	5.15/5.15	5.16
Rb-I/ Å	4.19	4.20	4.20	4.20	4.21
Sn/Te-I(equatorial)/ Å	2.90	2.90/2.96	2.90/2.96	2.90/2.96	2.96
Sn/Te-I(apical)/ Å	2.90	2.90/2.96	2.90/2.96	2.90.2.96	2.96
I- Sn/Te-I (equatorial)/˚	180˚	180˚	180˚	180˚	180˚
I- Sn/Te-I (apical)/˚	180˚	180˚	180˚	180˚	180˚

Table S2. Calculated tolerance factor t_{eff} and octahedral factor μ_{eff} for $Rb_2Sn_{1-x}Te_xI_6$ ($0 \leq x \leq 1$).

	t_{eff}	μ_{eff}
0% Te (Rb_2SnI_6)	0.96	0.31
25% Te ($Rb_2Sn_{0.75}Te_{0.25}I_6$)	0.94	0.35
50% Te ($Rb_2Sn_{0.50}Te_{0.50}I_6$)	0.92	0.38
75% Te ($Rb_2Sn_{0.25}Te_{0.75}I_6$)	0.89	0.41
100% Te (Rb_2TeI_6)	0.87	0.44

Table S3. Competing phases considered in calculating the chemical potential space of Rb_2SnI_6 and Rb_2TeI_6 along with their corresponding formation energies in eV.

Limits	ΔH	Limits	ΔH
RbSn	-0.612	Rb_2Te	-2.998
$RbSn_3$	-0.647	Rb_2Te_3	-3.584
RbI	-3.094	Rb_2Te_5	-3.772
RbI_3	-3.396	TeI	-0.252
SnI_2	-1.711	Te_2I	-0.255
SnI_4	-2.1835	TeI_4	-0.918
$RbSnI_3$	-4.950	Rb_2SnTe_3	-4.226
RbTe	-1.676		

Table S4. Band gaps of $Rb_2Sn_{1-x}Te_xI_6$ ($0 \leq x \leq 1$) calculated at different levels of theory along with experimental values.

Compound	$E_{g(PBE)}/eV$	$E_{g(mBJ)}/eV$	$E_{g(HSE)}/eV$	Other cal.	Exp:
Rb_2SnI_6	0.13	0.75	1.10	1.13[5]* /1.02[6]	1.32[5]
$Rb_2Sn_{0.75}Te_{0.25}I_6$	0.64	1.12	1.35		
$Rb_2Sn_{0.50}Te_{0.50}I_6$	0.72	1.19	1.44		
$Rb_2Sn_{0.25}Te_{0.75}I_6$	1.06	1.46	1.67		
Rb_2TeI_6	1.78	2.14	2.18		

*Band gap calculated for tetragonal phase of Rb_2SnI_6

Table S5. Calculated elastic constants (in GPa), Bulk moduli (in GPa), Shear moduli (in GPa), Young's moduli (in GPa), Passion's ratio (ν), Anisotropy factor (A), and Pugh's ratio, of $Rb_2Sn_{1-x}Te_xI_6$.

Compounds	C_{11}	C_{12}	C_{44}	C_{11}–C_{44}	B	G	E	ν	A	B/G
Rb_2SnI_6	116.56	65.30	60.10	5.19	82.39	83.31	186.93	0.12	2.34	0.98
$Rb_2Sn_{0.75}Te_{0.25}I_6$	98.51	52.27	40.74	11.53	67.68	61.69	141.95	0.15	1.76	1.09
$Rb_2Sn_{0.50}Te_{0.50}I_6$	109.27	63.73	47.01	16.71	78.91	73.36	168.02	0.14	2.06	1.07
$Rb_2Sn_{0.25}Te_{0.75}I_6$	101.19	61.65	39.45	22.19	74.83	66.63	154.15	0.16	1.99	1.13
Rb_2TeI_6	113.92	51.27	44.22	7.04	72.15	64.18	148.51	0.16	1.41	1.12

References

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