Electronic Supplementary Material (ESI) for Materials Horizons.

Supporting Information

Searching for promising new perovskite-based photovoltaic absorbers: the importance of electronic dimensionality

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Table S1. Experimental structural data (i.e., space group and structural dimensionality), and bandgaps (E_g) of some iodide perovskites and non-perovskites.

Compound[a]	Space group	*D*	E_g (eV)[b]
$(C_1)PbI_3$	*I4/mcm*[1]	3	1.52[2]
$CsPbI_3$	*Pm*-3*m*[3]	3	1.67[2]
$(C_1)SnI_3$	*P4mm*[2]	3	1.20[2]
$CsSnI_3$	*Fm*−3*m*[2]	3	1.30[2]
$(C_1)GeI_3$	*R*3*m*[4]	3	1.9[4]
$CsGeI_3$	*R*3*m*[4]	3	1.6[4]
$(C_6)_2PbI_4$	*Pbca*[5]	2	2.7*[6]
$(C_9)_2PbI_4$	*Pbca*[7]	2	2.82*[8]
$(C_{12})_2PbI_4$	*Pbca*[7]	2	2.88*[7]
$(C_1)_2Pb(SCN)_2I_2$	*Pnm*2_1[9]	2	2.3*[10]
$(C_{6\text{-}2})_2PbI_4$	*C*2/*m*[11]	2	2.57*[12]
$(C_1)(C_{6\text{-}2})_2Pb_2I_7$	*P*–1[11]	3 – 1/2	2.32*[12]
$(C_1)_2(C_{6\text{-}2})_2Pb_3I_{10}$	*P*1[13]	3 – 1/3	2.1*[13]
$(C_1)_5(C_{6\text{-}2})_2Pb_6I_{13}$	—	3 – 1/6	1.64[14]
$(C_1)_9(C_{6\text{-}2})_2Pb_{10}I_{31}$	—	3 – 1/10	1.624[14]
$(C_1)_{39}(C_{6\text{-}2})_2Pb_{40}I_{121}$	—	3 – 1/40	1.615[14]
$(C_1)_{59}(C_{6\text{-}2})_2Pb_{60}I_{181}$	—	3 – 1/60	1.613[14]
$(C_{6\text{-}2})_2SnI_4$	*C*2/*m*[15]	2	2.19*[15]
$Rb_3Bi_2I_9$	*P*2_1/*n*[16]	3 – 1/2	2.1[16]
$Cs_3Sb_2I_9$	*P*–3*m*1[17]	3 – 1/2	2.05[17]
δ-$CsPbI_3$	*Pnma*[3]	2 – 1/2	3.17*[18]
$(C_1I)PbI_5$	*P*2_1/*c*[19]	1	3.18*[20]
$(C_1I)SnI_5$	*P*2_1/*c*[19]	1	3.02*[8]
$(C_1)_3Bi_2I_9$	*P*6_3/*mmc*[21]	1 – 1/2	2.9*[21]
$Cs_3Bi_2I_9$	*P*6_3/*mmc*[22]	1 – 1/2	2.86*[23]
$(C_1)_4PbI_6{\cdot}2H_2O$	*P*2_1/*n*[24]	0	3.87*[8]
$(C_1)_4SnI_6{\cdot}2H_2O$	*P*2_1/*n*[24]	0	3.54*[8]

[a]"C_n" indicates $C_nH_{2n+1}NH_3$, "$C_{6\text{-}2}$" indicates $C_6H_5(CH_2)_2NH_3$, and "C_1I" indicates $NH_2C(I){=}NH_2$. [b]The "*" symbol indicate that the sub-gap excitonic band was excluded and the bandgap was determined from fundamental absorption band edge.

Table S2. Highest recorded PEC for some perovskites and non-perovskites with corresponding device open-circle voltage (V_{oc}), short-circuit current (J_{sc}) and fill factor (FF) data.

Compound[a]	PEC (%)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Ref.
$(C_1)PbI_3$	19.1	1.09	22.4	80	25
$(C_1,FA,Cs)PbI_3$	21.1	1.15	23.5	78	26
(FA)PbI3	20.1	1.06	24.7	78	27
$CsPbI_3$	2.9	0.80	12.0	—	28
$(C_1)SnI_3$	6.4	0.88	16.8	42	29
$(FA)SnI_3$	4.8	0.32	23.7	63	30
$CsSnI_3$	2.0	0.24	22.7	37	31
$(C_{6\text{-}2})(C_1)_{59}Pb_{60}I_{181}$	15.4	1.09	19.1	74	14
⊥-$(C_4)_2(C_1)_3Pb_4I_{13}$	12.5	1.01	16.8	74	32
⊥-$(C_4)_2(C_1)_2Pb_3I_{10}$	11.4	1.06	14.4	75	32
-$(C_4)_2(C_1)_3Pb_4I_{13}$	2.4	0.87	9.1	30	33
-$(C_4)_2(C_1)_2Pb_3I_{10}$	4.0	0.93	9.4	46	33
-$(C_{6\text{-}2})_2(C_1)_2Pb_3I_{10}$	4.7	1.18	6.7	60	13
-$(C_1)_2Pb(SCN)_2I_2$	3.2	0.65	6.8	73	34
-$(HA)_2PbI_4$	1.1	0.91	2.6	47	35
$Cs_3Sb_2I_9$	<0.1	0.31	—	—	17
$Cs_3Bi_2I_9$	1.1	0.85	2.2	60	36
$(C_1)GeI_3$	0.20	0.15	4.0	30	37
$CsGeI_3$	0.11	0.07	5.7	27	37

[a]"C_n" indicates $C_nH_{2n+1}NH_3$, "$C_{6\text{-}2}$" indicates $C_6H_5(CH_2)_2NH_3$, "C_1I" indicates $NH_2C(I){=}NH_2$, "FA" indicates $HC(NH_2)_2$, and "HA" indicates $C_5N_3H_{11}$. The " " and "⊥" symbols indicate that the films are grown with the layers parallel to and perpendicular to the substrates, respectively.

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