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Supplementary Information

A DFT study on the stability and optoelectronic property of Pb/Sn/Ge-based $MA_2B(SCN)_2I_2$ perovskites

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Table S1. Relative energies for the hybrid structures of $MA_2Pb_{1-x}Sn_x(SCN)_2I_2$ (x = 0.25, 0.50, 0.75) with different doping sites.

System	Doping site	Relative energies (eV)
x = 0.25	1	0
	2	0.015
	3	0.011
	4	0.027
x = 0.50	1	0
	2	0.048
	3	0.006
	4	0.040
	5	0.037
	6	0.031
x = 0.75	1	0
	2	0.010
	3	0.026

Table S2. Atomic coordinates of H, C, N, S, I and Pb elements in $MA_2Pb(SCN)_2I_2$ structure.

			x	**y**	**z**	**Wyckoff Position**
1	H	H1	0.299	0.543	0.702	4b
2	H	H2	0.320	0.469	0.539	4b
3	H	H3	0.371	0.546	0.620	4b
4	H	H4	0.376	0.464	0.923	4b
5	H	H5	0.393	0.381	0.747	4b
6	H	H6	0.316	0.385	0.848	4b
7	H	H7	0.201	0.043	0.202	4b
8	H	H8	0.180	0.031	0.039	4b

9	H	H9	0.129	0.056	0.120	4b
10	H	H10	0.124	0.036	0.423	4b
11	H	H11	0.107	0.119	0.247	4b
12	H	H12	0.184	0.115	0.348	4b
13	H	H13	0.799	0.043	0.202	4b
14	H	H14	0.820	0.031	0.039	4b
15	H	H15	0.871	0.046	0.120	4b
16	H	H16	0.876	0.036	0.423	4b
17	H	H17	0.893	0.119	0.247	4b
18	H	H18	0.816	0.115	0.348	4b
19	H	H19	0.701	0.543	0.702	4b
20	H	H20	0.680	0.469	0.539	4b
21	H	H21	0.629	0.546	0.620	4b
22	H	H22	0.624	0.464	0.923	4b
23	H	H23	0.607	0.381	0.747	4b
24	H	H24	0.684	0.385	0.848	4b
25	H	H25	0.299	1.043	0.702	4b
26	H	H26	0.320	0.969	0.539	4b
27	H	H27	0.371	1.046	0.620	4b
28	H	H28	0.376	0.964	0.923	4b
29	H	H29	0.393	0.881	0.747	4b
30	H	H30	0.316	0.885	0.848	4b
31	H	H31	0.201	0.457	0.202	4b
32	H	H32	0.180	0.531	0.039	4b
33	H	H33	0.129	0.454	0.120	4b
34	H	H34	0.124	0.536	0.423	4b
35	H	H35	0.107	0.619	0.247	4b
36	H	H36	0.184	0.615	0.348	4b
37	H	H37	0.799	0.457	0.202	4b

38	H	H38	0.820	0.531	0.039	4b
39	H	H39	0.871	0.454	0.120	4b
40	H	H40	0.876	0.536	0.423	4b
41	H	H41	0.893	0.619	0.247	4b
42	H	H42	0.816	0.615	0.348	4b
43	H	H43	0.701	1.043	0.702	4b
44	H	H44	0.680	0.969	0.539	4b
45	H	H45	0.629	1.046	0.620	4b
46	H	H46	0.624	0.964	0.923	4b
47	H	H47	0.607	0.881	0.747	4b
48	H	H48	0.684	0.885	0.848	4b
49	C	C1	0.311	0.281	0.268	4b
50	C	C2	0.357	0.427	0.805	4b
51	C	C3	0.190	0.219	0.768	4b
52	C	C4	0.143	0.073	0.305	4b
53	C	C5	0.190	0.219	0.768	4b
54	C	C6	0.857	0.073	0.305	4b
55	C	C7	0.689	0.281	0.268	4b
56	C	C8	0.643	0.427	0.805	4b
57	C	C9	0.311	0.781	0.268	4b
58	C	C10	0.357	0.927	0.805	4b
59	C	C11	0.190	0.719	0.768	4b
60	C	C12	0.143	0.573	0.305	4b
61	C	C13	0.190	0.719	0.768	4b
62	C	C14	0.857	0.573	0.305	4b
63	C	C15	0.689	0.781	0.268	4b
64	C	C16	0.643	0.927	0.805	4b
65	N	N1	0.287	0.366	0.297	4b
66	N	N2	0.334	0.503	0.652	4b

67	N	N3	0.213	0.134	0.797	4b
68	N	N4	0.166	0.003	0.152	4b
69	N	N5	0.213	0.134	0.797	4b
70	N	N6	0.834	0.003	0.152	4b
71	N	N7	0.713	0.366	0.297	4b
72	N	N8	0.666	0.503	0.652	4b
73	N	N9	0.287	0.866	0.297	4b
74	N	N10	0.334	1.003	0.652	4b
75	N	N11	0.213	0.634	0.797	4b
76	N	N12	0.166	0.497	0.152	4b
77	N	N13	0.213	0.634	0.797	4b
78	N	N14	0.834	0.497	0.152	4b
79	N	N15	0.713	0.866	0.297	4b
80	N	N16	0.666	1.003	0.652	4b
81	S	S1	0.342	0.164	0.229	4b
82	S	S2	0.158	0.336	0.729	4b
83	S	S3	0.158	0.336	0.729	4b
84	S	S4	0.658	0.164	0.229	4b
85	S	S5	0.342	0.664	0.229	4b
86	S	S6	0.158	0.836	0.729	4b
87	S	S7	0.158	0.836	0.729	4b
88	S	S8	0.658	0.664	0.229	4b
89	I	I1	0.500	0.446	0.277	2a
90	I	I2	0.500	0.181	0.742	2a
91	I	I3	0.000	0.054	0.777	2a
92	I	I4	0.000	0.319	0.242	2a
93	I	I5	0.500	0.946	0.277	2a
94	I	I6	0.500	0.681	0.742	2a
95	I	I7	0.000	0.554	0.777	2a

96	I	I8	0.000	0.819	0.242	2a
97	Pb	Pb1	0.500	0.196	0.234	2a
98	Pb	Pb2	0.000	0.304	0.734	2a
99	Pb	Pb3	0.500	0.696	0.234	2a
100	Pb	Pb4	0.000	0.804	0.734	2a

Table S3. Average interatomic distances B-I and B-S (in Å) for $MA_2B(SCN)_2I_2$ (B = Pb, Sn, Ge) and $MA_2Pb_{1-x}Sn_x(SCN)_2I_2$ (x = 0.25, 0.50, 0.75) perovskites.

	Apical			Equatorial			B-S		
system	Pb-I	Sn-I	Ge-I	Pb-I	Sn-I	Ge-I	Pb-S	Sn-S	Ge-S
B = Pb	3.204			3.321			3.019		
B = Sn		3.173			3.322			2.947	
B = Ge			3.123			3.315			2.785
x = 0.25	3.204	3.165		3.338	3.336		3.010	2.954	
x = 0.50	3.202	3.199		3.349	3.343		3.012	2.953	
x = 0.75	3.216	3.175		3.349	3.343		3.012	2.959	

Table S4. Calculated bond angles of B-I-B (º) along the x-y plane for $MA_2B(SCN)_2I_2$ (B = Pb, Sn, Ge) and $MA_2Pb_{1-x}Sn_x(SCN)_2I_2$ (x = 0.25, 0.50, 0.75) perovskites.

system	Pb-I-Pb	Sn-I-Sn	Ge-I-Ge
B = Pb	164.710		
B = Sn		163.431	
B = Ge			159.498
x = 0.25	164.263		
x = 0.50	163.855	164.667	
x = 0.75		164.036	

Table S5. Total energy of decomposed fragments after optimized for $MA_2B(SCN)_2I_2$ (B = Pb, Sn, Ge) and $MA_2Pb_{1-x}Sn_x(SCN)_2I_2$ (x = 0.25, 0.50, 0.75).

System	Com.	E(eV)	Com.	E(eV)	Com.	E(eV)
B = Pb	2MAI	-84.918	$Pb(SCN)_2$	-46.265	-	-
B = Sn	2MAI	-84.918	$Sn(SCN)_2$	-46.374	-	-
B = Ge	2MAI	-84.918	$Ge(SCN)_2$	-45.082	-	-

x = 0.25	2MAI	-84.918	0.75Pb(SCN)$_2$	-34.699	0.25Sn(SCN)$_2$	-11.594
x = 0.50	2MAI	-84.918	0.50Pb(SCN)$_2$	-23.133	0.50Sn(SCN)$_2$	-23.187
x = 0.75	2MAI	-84.918	0.25Pb(SCN)$_2$	-11.566	0.75Sn(SCN)$_2$	-34.781

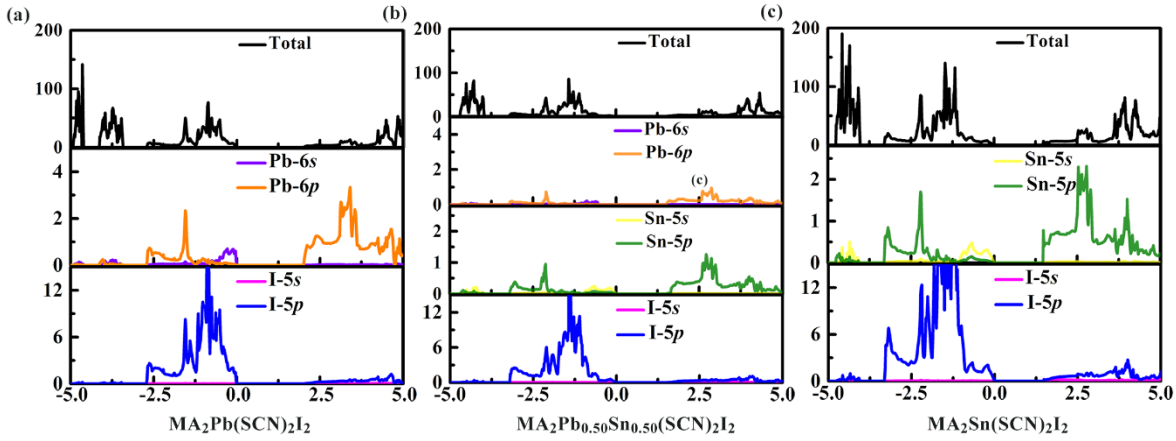

Figure S1. Respective PDOS of Pb, Sn and I atoms for (a) $MA_2Pb(SCN)_2I_2$, (b) $MA_2Pb_{0.50}Sn_{0.50}(SCN)_2I_2$, and (c) $MA_2Sn(SCN)_2I_2$ compounds.