Supplementary Materials

Table S1: Absorption and emission energies without applied strain, calculated considering spin-orbit coupling effects.

	Absorption (eV)	Emission (eV)
Sn	2.65	2.33
Pb	2.78	0.99

By comparing with experimental results, we found that the calculations without considering spin-orbit coupling (SOC) align more closely with the experimental observations. This could be due to the complexity of experimental conditions, where factors such as temperature effects, defects, and impurities in the material may partially mitigate the influence of SOC. Furthermore, approximations in the theoretical calculations might lead to an overestimation of the SOC effect, resulting in discrepancies between the computational and experimental values. For these reasons, we believe that in the current study, the calculations excluding SOC more accurately reflect the optical behavior observed in experiments. Therefore, we primarily report the computational results without SOC in the main text.

Table S2: Experimental and calculated lattice parameters of $(C_4N_2H_{14})PbBr_4$ and $(C_4N_2H_{14})SnBr_4$.

Parameter	a (Å)	b (Å)	c (Å)
$(C_4N_2H_{14})PbBr_4$ (Calc.)	6.072	14.361	14.067
$(C_4N_2H_{14})PbBr_4$ (exp.) [1]	6.104	14.623	14.407
$(C_4N_2H_{14})SnBr_4$ (Calc.)	6.114	14.502	14.322
$(C_4N_2H_{14})SnBr_4$ (exp.) [2]	6.114	14.502	14.322

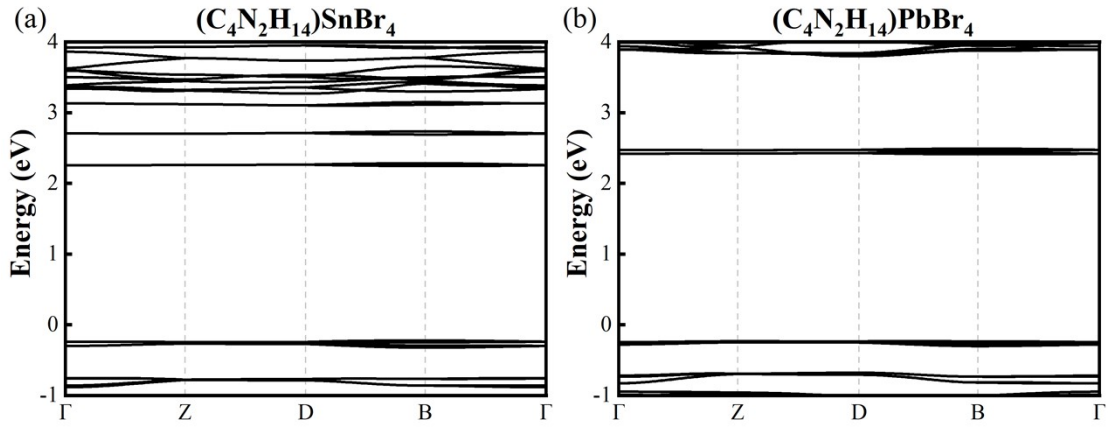

Figure S1: (a) Band structure of $(C_4N_2H_{14})SnBr_4$; (b) Band structure of $(C_4N_2H_{14})PbBr_4$.

Table S3. Effective masses of $C_4N_2H_{14}SnBr_4$ and $C_4N_2H_{14}PbBr_4$ considering third- and fourth-order corrections.

	$C_4N_2H_{14}SnBr_4$			$C_4N_2H_{14}PbBr_4$		
Strain (%)	m_x	m_y	m_z	m_x	m_y	m_z
-2	0.23	23.23	16.41	0.25	14.6	80.15
-1	0.25	22.11	33.63	0.27	15.7	90.41
0	0.26	21.61	59.34	0.29	16.1	116.1
1	0.29	20.42	35.1	0.32	16.5	120.4
2	0.32	19.11	44.1	0.34	19.3	100.6

References

1.Angew. Chem. Int. Ed. 2017, 56, 9018 –9022

2.Nat Commun 8, 14051 (2017)