Supporting Information

A Chiral Lead-Free Photoactive Hybrid Material with a Narrow Band Gap

Yaobin Li,[a,b] Tao Yang,[a] Xitao Liu,[a,c] Shiguo Han, [a] Jiaqi Wang, [a] Yu Ma, [a] Wuqian Guo, [a] Junhua Luo [a] and Zhihua Sun *[a,c]

[a.] State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, P. R. China

[b.] College of Chemistry and Materials Science, Fujian Normal University, Fuzhou, Fujian 350007, P. R. China

[c.] Universities of the Chinese Academy of Sciences, Beijing 100039, P. R. China

***Correspondence:** sunzhihua@fjirsm.ac.cn

Table of Contents:

Figure:

Table:

Figure

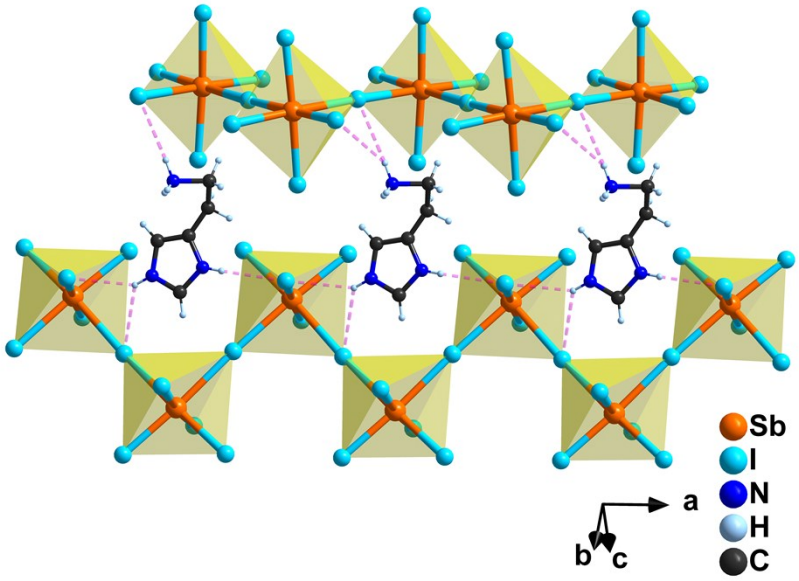

Figure S1. Crystal structure of **1.**.

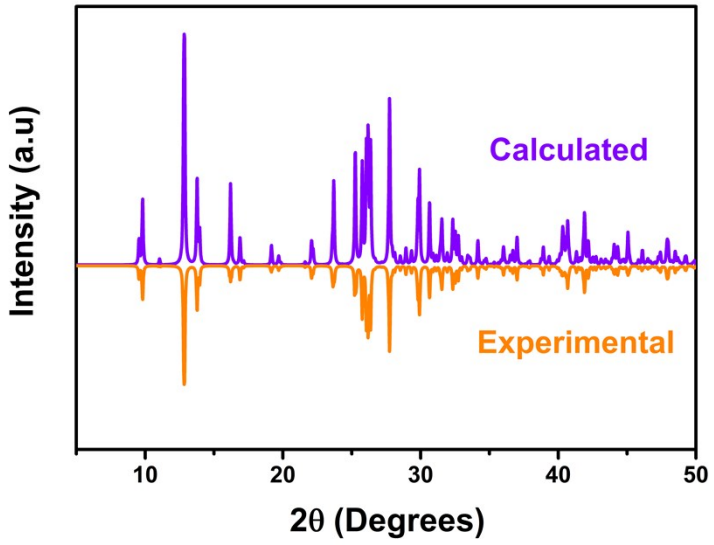

Figure S2. Experimental and simulated X-ray powder diffraction patterns for **1**.

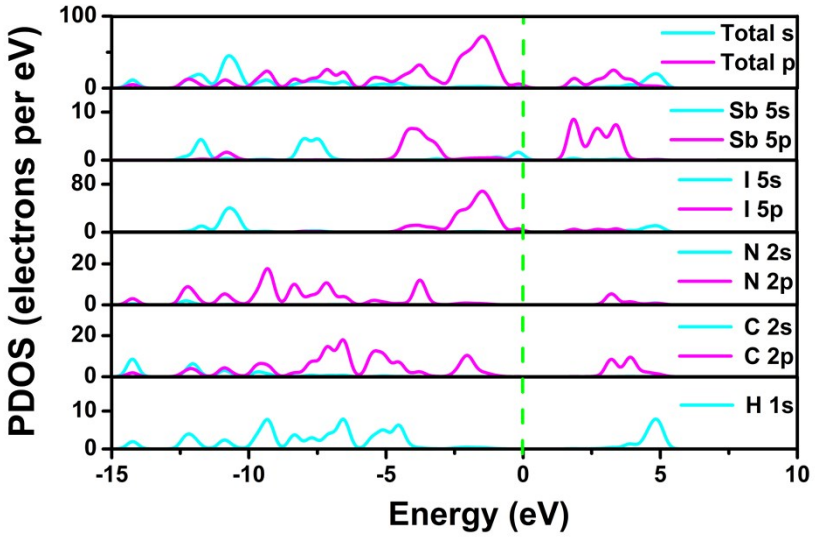

Figure S3. Partial density of states (PDOS) of **1**.

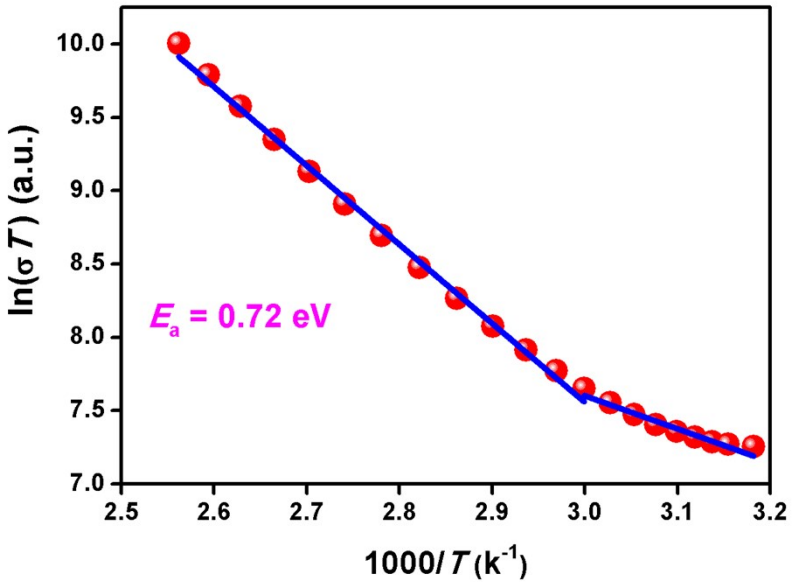

Figure S4. Arrhenius plot relating to the dependence of conductivity on temperature

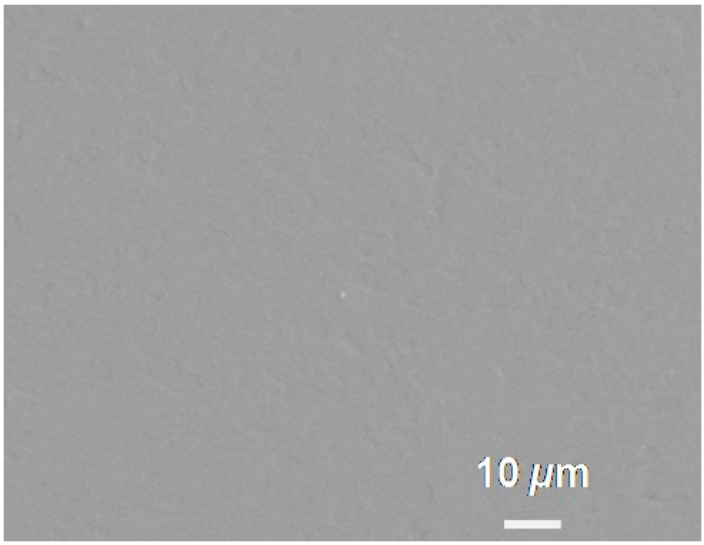

Figure S5. SEM images of crystal surface for **1**.

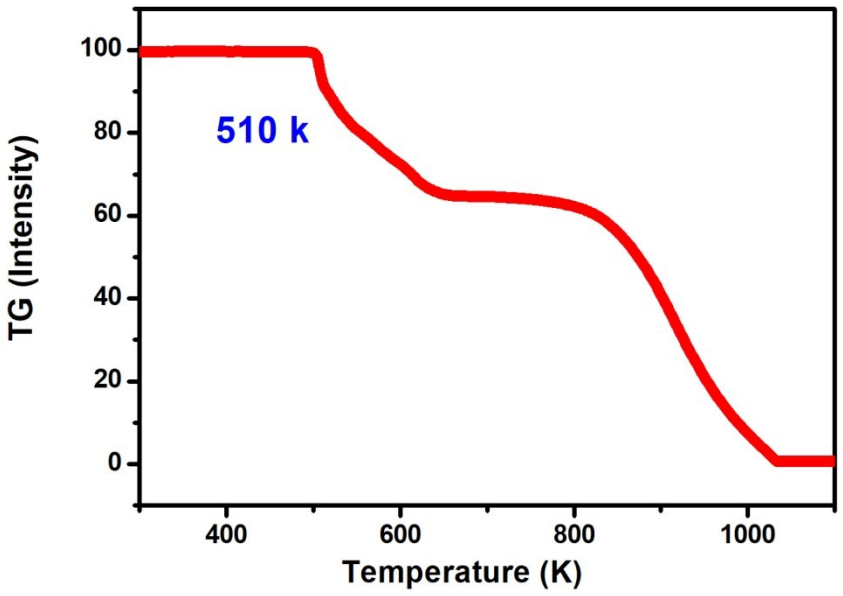

Figure S6. Thermogravimetric (TG) curve of **1**.

Table S1. Crystal data for 1

Empirical formula	$C_5H_{11}I_5N_3Sb$
Formula weight	869.42
Temperature/K	320.02
Crystal system	orthorhombic
Space group	$P2_12_12_1$
Cell parameters	a = 8.9312(2)
	b = 10.7807(3)
	c = 18.0106(6)
	β = 90
	V = 1734.14(8)
Z, Calculated density	4, 3.330 g/cm3
F(000)	1512.0
Radiation	Mo$K\alpha$ (λ = 0.71073)
Theta range	4.404 to 54.276°
	-11 ≤ h ≤ 11,
Limiting indices	-13 ≤ k ≤ 6,
	-28 ≤ l ≤ 21
Reflections collected / unique	14571/3823 (R_{int} = 0.0529)
Data/restraints/parameters	3823/99/120
GOF.	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0521, ωR_2 = 0.1282
R indexes (all data)	R_1 = 0.0711, ωR_2 = 0.1431

Table S2. Bond lengths for 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Sb1	I2	2.8952(8)	N1	C1	1.4200
Sb1	I1	3.0008(8)	C2	C3	1.4200
Sb1	I3	2.8604(8)	C3	N2	1.4200
Sb1	I5	3.1750(8)	C3	C4	1.446(11)
Sb1	$I5^{\#1}$	3.2270(8)	N2	C1	1.4200
Sb1	I4	3.0371(8)	C4	C5	1.435(12)
N1	C2	1.4200	N3	C5	1.456(12)

#1 -1/2+X,3/2-Y,1-Z

Table S3. Bond angles for 1.

Bond	Angle/˚	Bond	Angle/˚
I2-Sb1-I1	90.27(2)	I4-Sb1-I5	88.51(2)
I2-Sb1-I5	176.75(3)	I4-Sb1-I51	88.91(2)
$I2\text{-}Sb1\text{-}I5^{\#1}$	88.83(2)	$Sb1\text{-}I5\text{-}Sb1^{\#2}$	176.71(3)
I2-Sb1-I4	89.52(2)	C2-N1-C1	108.0
$I1\text{-}Sb1\text{-}I5^{\#1}$	87.51(2)	N1-C2-C3	108.0
I1-Sb1-I5	91.53(2)	C2-C3-N2	108.0
I1-Sb1-I4	176.42(3)	C2-C3-C4	136.9(9)
I3-Sb1-I2	94.64(2)	N2-C3-C4	115.0(9)
I3-Sb1-I1	92.42(2)	C1-N2-C3	108.0
$I3\text{-}Sb1\text{-}I5^{\#1}$	176.53(3)	N2-C1-N1	108.0
I3-Sb1-I5	87.98(2)	C5-C4-C3	145.1(11)
I3-Sb1-I4	91.16(2)	C4-C5-N3	90.4(9)
$I5\text{-}Sb1\text{-}I5^{\#1}$	88.549(11)		

#1 -1/2+X,3/2-Y,1-Z; #2 1/2+X,3/2-Y,1-Z