

Supporting Information

A Lead-Free I-Based Hybrid Double Perovskite (I-C₄H₈NH₃)₄AgBiI₈ for X-ray Detection

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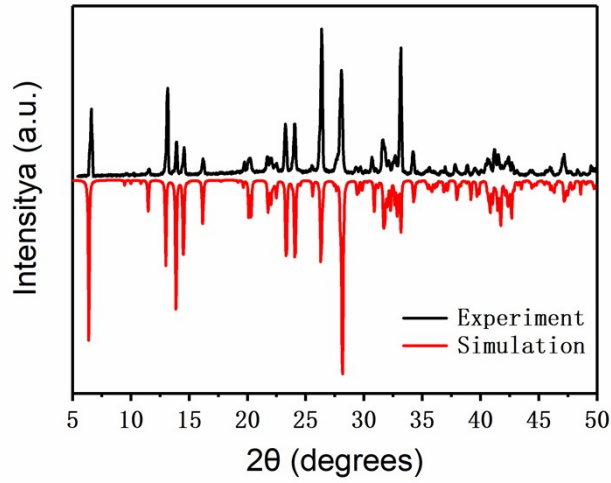


Figure S1. X-ray diffraction patterns for IAB

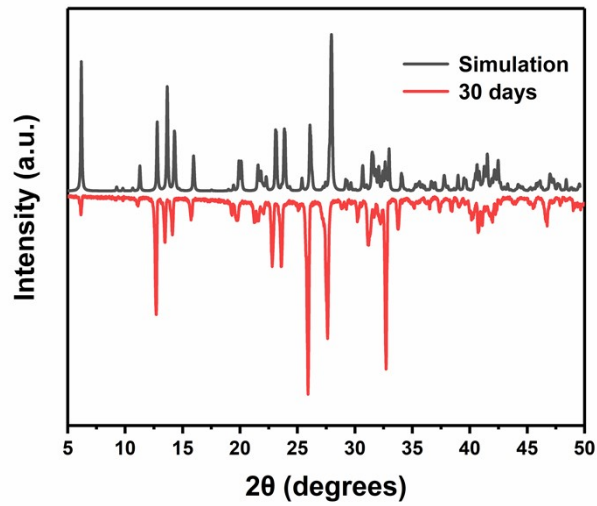


Figure S2. X-ray diffraction patterns for IAB after 30 days

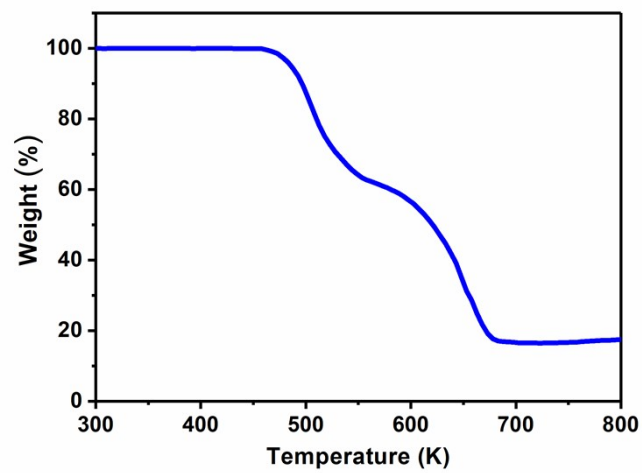


Figure S3. Thermogravimetric analysis of IAB.

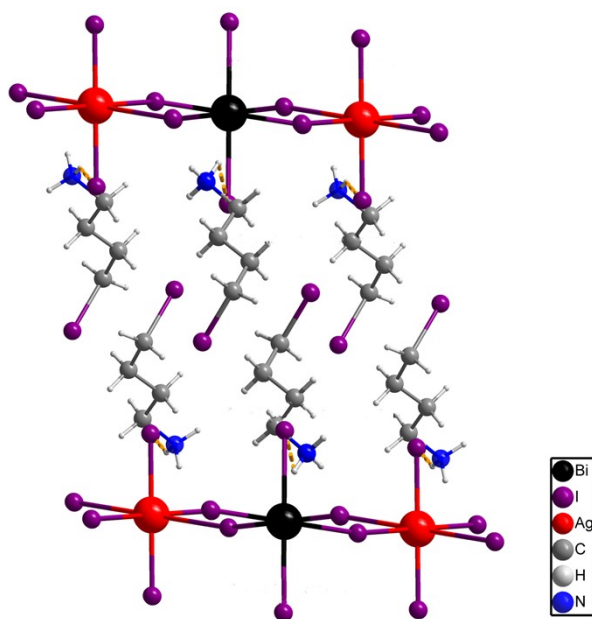


Figure S4. Hydrogen bonds in the compound **IAB** (Hydrogen bonds are represented by dotted lines).

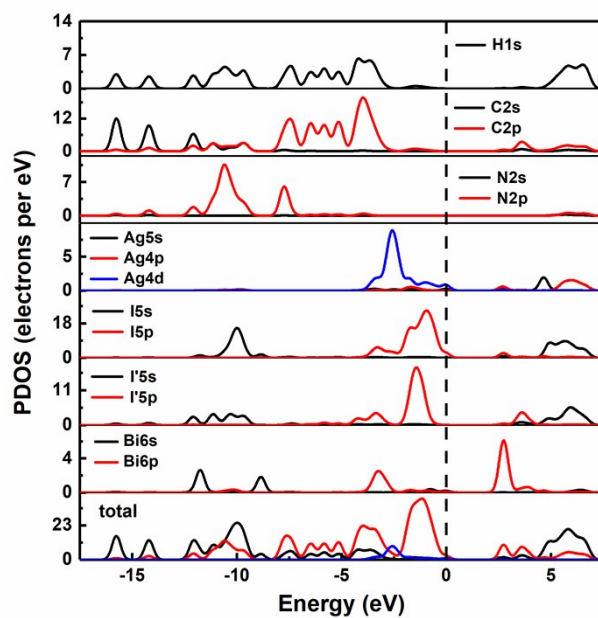


Figure S5. Partial density of states of **IAB**.

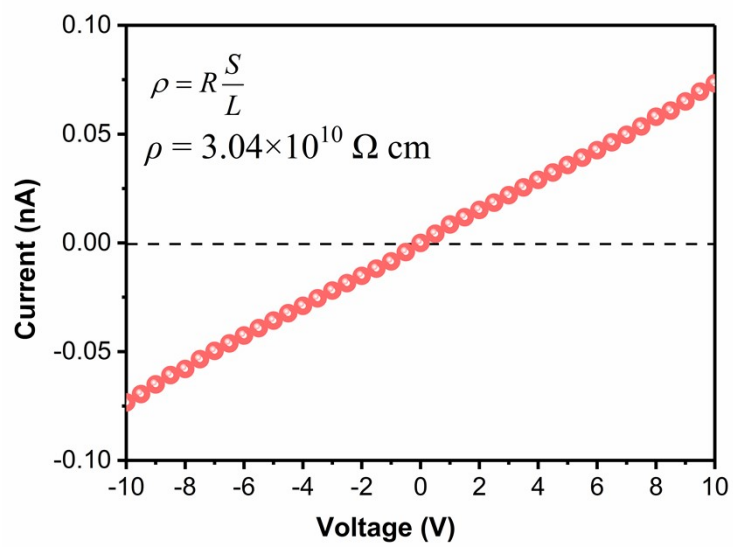


Figure S6. Bulk resistivity of IAB

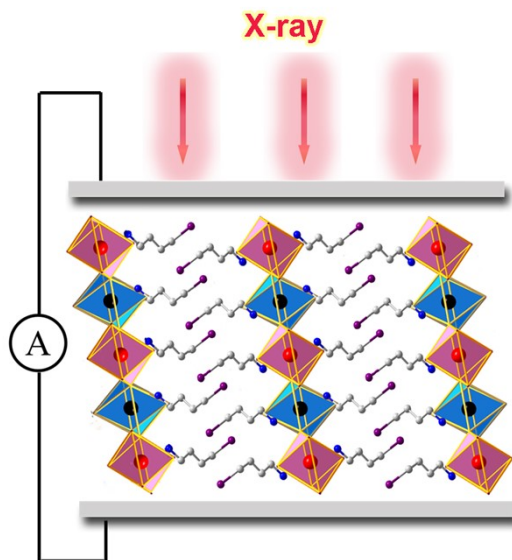


Figure S7. Schematic structure of the X-ray photoconductor based on the single crystal of IAB.

Table S1. Crystal data and structure refinement for **IAB**

Empirical formula	C ₁₆ H ₄₄ N ₄ AgBiI ₁₂
Formula weight	2132.2
Temperature/K	100.0
Crystal system	triclinic
Space group	<i>P</i> -1
<i>a</i> /Å	8.8214 (3)
<i>b</i> /Å	9.1445 (5)
<i>c</i> /Å	13.6531 (8)
α /°	89.767 (5)
β /°	79.205 (4)
γ /°	89.824 (4)
Volume/Å ³	1081.86 (10)
<i>Z</i>	1
ρ_{calc} g/cm ³	3.273
μ /mm ⁻¹	13.090
F(000)	934.0
Radiation	MoK α (λ = 0.71073)
Theta range (°)	6.786 to 59.47
Index ranges	-12 ≤ <i>h</i> ≤ 10, -12 ≤ <i>k</i> ≤ 11, -18 ≤ <i>l</i> ≤ 17
Reflections collected	12832
Independent reflections	8192 [<i>R</i> _{int} = 0.0546, <i>R</i> _{sigma} = 0.0520]
Data/restraints/parameters	5223/6/159
GOF	1.125
Final <i>R</i> indexes [<i>I</i> ≥ 2σ (<i>I</i>)]	<i>R</i> ₁ = 0.0456, <i>wR</i> ₂ = 0.1552
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0508, <i>wR</i> ₂ = 0.1605
CCDC number	2086155