

Supporting Information

Zero-dimensional indium hybrid and modulated photoluminescence by Sb doping

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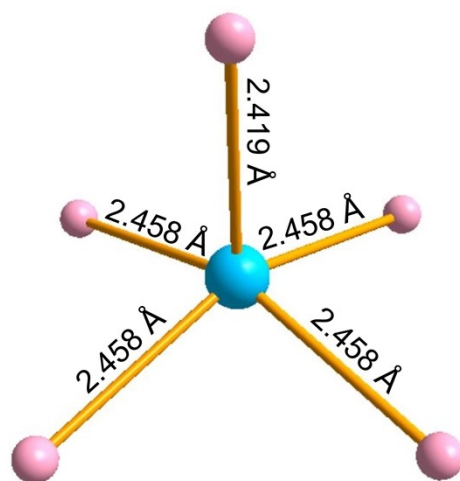


Fig. S1. The In-Cl bond lengths in the $[\text{InCl}_5]^{2-}$ square pyramid structure.

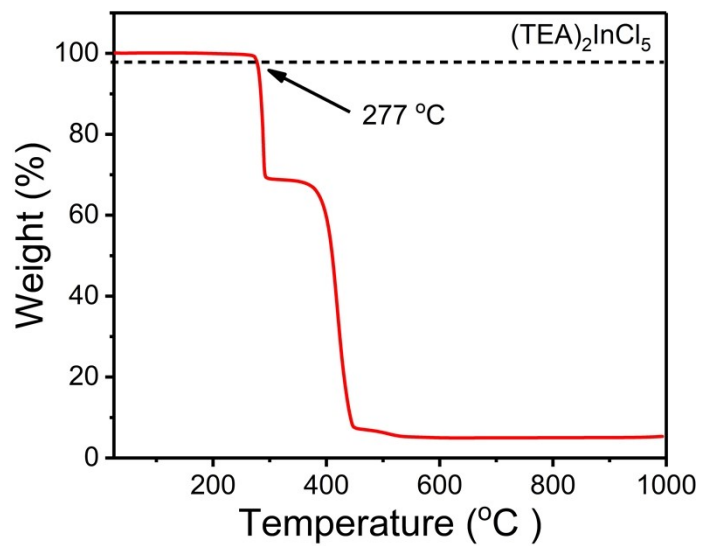


Fig. S2. The TGA data of the as-synthesized $(\text{TEA})_2\text{InCl}_5$.

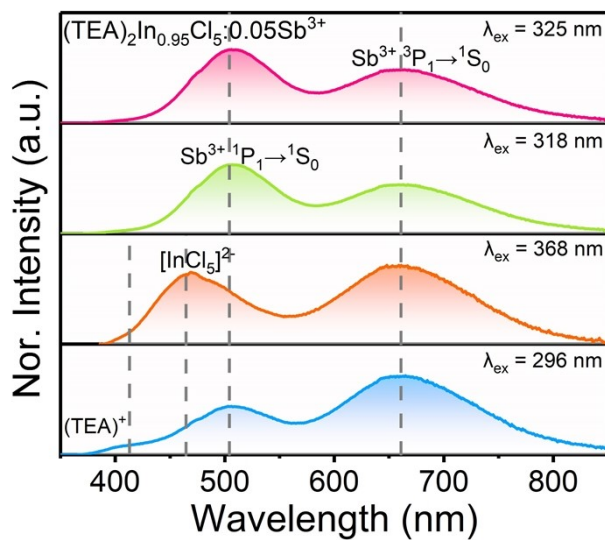


Fig. S3. Room-temperature PL spectra of $(\text{TEA})_2\text{In}_{0.95}\text{Cl}_5:0.05\text{Sb}^{3+}$.

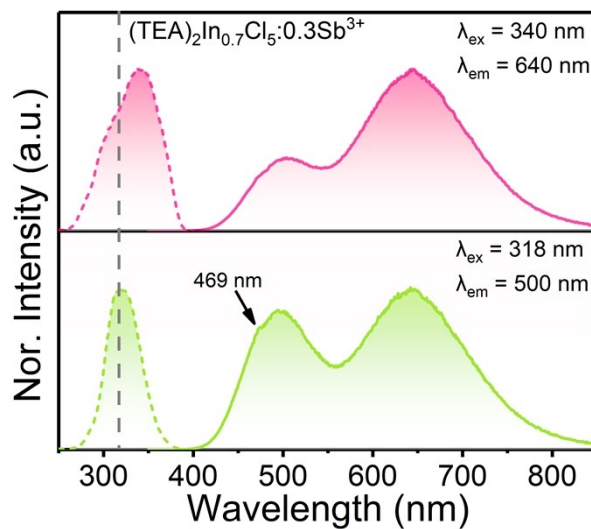


Fig. S4. The PL and PLE spectra of $(\text{TEA})_2\text{In}_{0.7}\text{Cl}_5:0.3\text{Sb}^{3+}$.

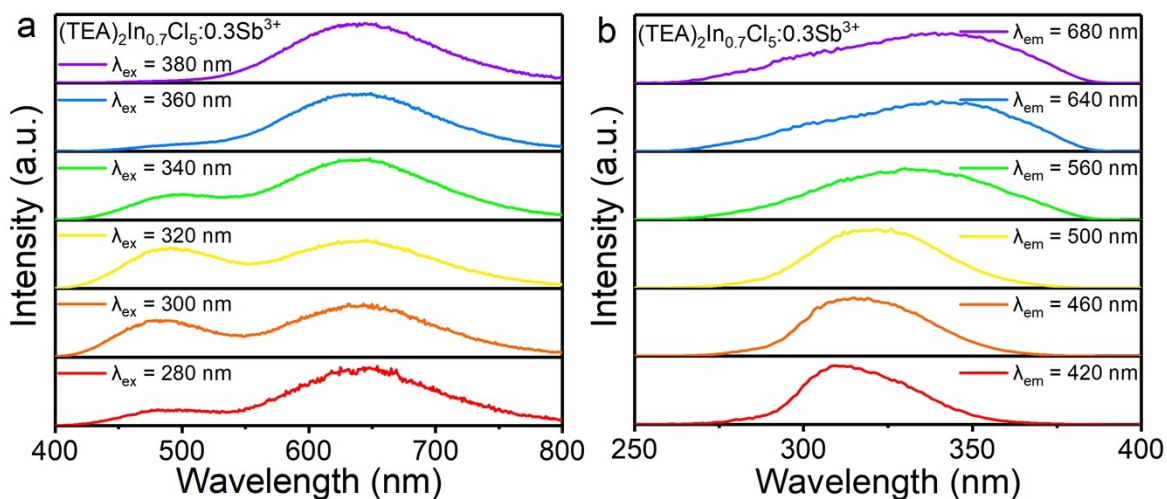


Fig. S5. Wavelength-dependent (a) PL and (b) PLE spectra of $(\text{TEA})_2\text{In}_{0.7}\text{Cl}_5:0.3\text{Sb}^{3+}$.

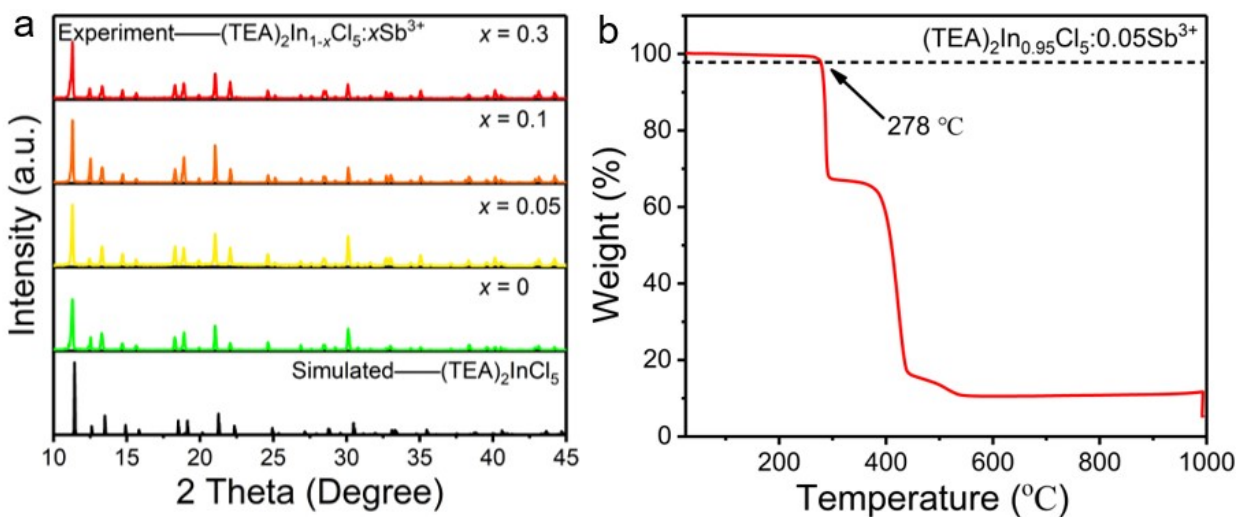


Fig. S6. (a) PXRD patterns of $(\text{TEA})_2\text{In}_{1-x}\text{Cl}_5:x\text{Sb}^{3+}$ after 90 days of exposure to light and moisture conditions. (b) The TGA data of $(\text{TEA})_2\text{In}_{0.95}\text{Cl}_5:0.05\text{Sb}^{3+}$.

Table S1. Comparison of structural and photoluminescent properties of the reported 0D In-based OIMHs.

Compound	Inorganic units	λ_{em} (nm)	PLQY (%)	Ref
(PMA) ₃ InBr ₆	[InBr ₆] ³⁻	610	35	1
(C ₈ NH ₁₂) ₆ InBr ₉ ·H ₂ O	[InBr ₆] ³⁻	475, 700	8.85	2
(PEA) ₄ NaInCl ₈	[InCl ₆] ³⁻	282	<1	3
(PEA) ₂ CsNaInCl ₇	[InCl ₆] ³⁻	282	<1	3
TpyInCl ₃	[InN ₃ Cl ₃] ³⁻	465, 575	6.06	4
InCl ₆ (C ₄ H ₁₀ SN) ₄ ·Cl	[InCl ₆] ³⁻	550	20	5
[DAPEDA]InCl ₆ ·Cl·H ₂ O	[InCl ₆] ³⁻	520	40.4	6
[DPA] ₃ InCl ₆	[InCl ₆] ³⁻	510	34.01	6
(C ₂ H ₈ N) ₄ InCl ₇	[InCl ₆] ³⁻	405, 620	13.9	7
AEPz-In	[InCl ₆] ³⁻	444, 538	1.38, 6.42	8
AMPd-In	[InCl ₆] ³⁻	443, 562	6.41, 19.02	8
PhPz-In	[InCl ₆] ³⁻	443, 575	20, 20.15	8
(CH ₃ NH ₃) ₄ InCl ₆ ·Cl	[InCl ₆] ³⁻	-	-	9
(C ₇ H ₈ N ₃) ₃ InCl ₆ ·H ₂ O	[InCl ₆] ³⁻	558	<1	10
(C ₇ H ₈ N ₃) ₃ InBr ₆ ·H ₂ O	[InBr ₆] ³⁻	595	5	10
TpyInCl ₅	[In ₂ Cl ₁₀] ³⁻	465	47.66	4
BAPPIIn ₂ Cl ₁₀	[In ₂ Cl ₁₀] ⁴⁻	440	8	11
(C ₄ H ₁₄ N ₂) ₂ In ₂ Br ₁₀	[InBr ₆] ³⁻ + [InBr ₄] ⁻	445, 670	3	12
(C ₁₁ H ₂₄ N ₂) ₂ [InBr ₆][InBr ₄]	[InBr ₆] ³⁻ + [InBr ₄] ⁻	660	8	13
RInBr ₄	[InBr ₄] ⁻	437, 451	16.36	14
(C ₂₀ H ₂₀ P) ₂ InCl ₅	[InCl ₅] ²⁻	-	-	15
(C ₆ H ₁₈ N ₂)InCl ₅ ·H ₂ O	[InCl ₅] ²⁻	-	-	16
(C ₁₃ H ₁₄ N) ₂ InCl ₅	[InCl ₅] ²⁻	435	5.44	17
(TEA) ₂ InCl ₅	[InCl ₅] ²⁻	468	30.11	This work

Table S2. Single crystal X-ray diffraction data and collection parameters. The collection was performed at a temperature of 150 K.

Empirical formula	$C_{16}H_{40}Cl_5InN_2$
Formula weight	552.57
Temperature/K	150.0
Crystal system	tetragonal
Space group	$P4/n$
$a/\text{\AA}$	9.2680(2)
$b/\text{\AA}$	9.2680(2)
$c/\text{\AA}$	14.0369(6)
α°	90
β°	90
γ°	90
Volume/ \AA^3	1205.71(7)
Z	2
$\rho_{\text{calc}}/\text{g/cm}^3$	1.522
μ/mm^{-1}	1.537
F(000)	568.0
Crystal size/ mm^3	0.2×0.15×0.1
Radiation	MoK α ($\lambda = 0.71073$)
2 θ range for data collection/ $^\circ$	2.902 to 52.718
Index ranges	$-11 \leq h \leq 11, -11 \leq k \leq 9, -17 \leq l \leq 17$
Reflections collected	11320
Independent reflections	1244 [$R_{\text{int}} = 0.0243, R_{\text{sigma}} = 0.0126$]
Data/restraints/parameters	1244/0/78
Goodness-of-fit on F^2	1.120
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0317, wR_2 = 0.0935$
Final R indexes [all data]	$R_1 = 0.0350, wR_2 = 0.0960$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	1.68/-0.60

Table S3. CIE chromaticity Coordinates and CCT for $(\text{TEA})_2\text{In}_{1-x}\text{Cl}_5:x\text{Sb}^{3+}$ under different conditions.

Sample No.	Composition	CIE (x, y)	CCT	λ_{ex} (nm)
1	$x = 0.3$	(0.483, 0.384)	2569	280
2	$x = 0.3$	(0.367, 0.330)	4054	318
3	$x = 0.3$	(0.397, 0.353)	3424	330
4	$x = 0.3$	(0.436, 0.376)	2918	340
5	$x = 0.3$	(0.547, 0.413)	2617	368
6	$x = 0$	(0.143, 0.111)	18113	368
7	$x = 0.05$	(0.345, 0.275)	4592	368
8	$x = 0.1$	(0.536, 0.394)	2659	368

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