

Supporting Information

Zn²⁺ and Cu²⁺ doping of one-dimensional lead free hybrid perovskite ABX₃: For white light emission and green solar cells applications

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Table S1. Crystal data and refinement parameters of DMACdCl₃, DMACdCl₃ : Zn and DMACdCl₃ : Cu

	DMACdCl₃	DMACdCl₃ : Zn	DMACdCl₃ : Cu
Empirical formula	(CH ₃) ₂ NH ₂ CdCl ₃	(CH ₃) ₂ NH ₂ Cd _{0.98} Zn _{0.02} Cl ₃	(CH ₃) ₂ NH ₂ Cd _{0.97} Cu _{0.03} Cl ₃
Formula weight (g/mol ⁻¹)	264.85	263.9	263.43
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
Crystal system	Monoclinic	Monoclinic	Monoclinic
<i>a</i> (Å)	8.758(2)	8.739(11)	8.750(10)
<i>b</i> (Å)	13.289(3)	13.281(18)	13.279(15)
<i>c</i> (Å)	6.694(3)	6.694(8)	6.689(7)
β (°)	98.371(10)	98.367(5)	98.293(4)
<i>V</i> (Å ³)	770.91(4)	768.76(17)	769.22(15)
<i>Z</i>	4	4	4
Cell measurement temperature (°C)	296(2)	296(2)	293(2)
Crystal size (mm ³)	0.39 × 0.28 × 0.017	0.320 × 0.270 × 0.180	0.400 × 0.240 × 0.140
Crystal color and shape	Colorless stick	Colorless stick	Yellow stick
λ (MoKα) (Å)	0.71073	0.71073	0.71073
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Transmission factors	0.246 , 0.930	0.129 , 0.293	0.313 , 0.620
hkl range	-13 ≤ <i>h</i> ≤ 13 -20 ≤ <i>k</i> ≤ 20 -10 ≤ <i>l</i> ≤ 10	-11 ≤ <i>h</i> ≤ 11 -17 ≤ <i>k</i> ≤ 15 -8 ≤ <i>l</i> ≤ 8	-11 ≤ <i>h</i> ≤ 11 -17 ≤ <i>k</i> ≤ 17 -8 ≤ <i>l</i> ≤ 7
Programs system	SHELXL-2018	SHELXL-2018	SHELXL-2018
θ range for data collection (deg)	3.44 - 37.95	2.280 - 27.514	3.068 - 27.491
Diffractometer	D8 VENTURE Bruker AXS	D8 VENTURE Bruker AXS	D8 VENTURE Bruker AXS
No. of reflection	17697	7623	6570

collected			
No. of independent reflection	2755	1766	1769
No. of reflections observed ($I > 2\sigma(I)$)	2587	1616	1610
No. of parameters	121	68	68
Goodness of fit	1.085	1.14	1.133
R indices ($I > 2\sigma(I)$)	$R_1 = 0.0182$ $wR_2 = 0.0395$	$R_1 = 0.0239$ $wR_2 = 0.0566$	$R_1 = 0.0272$ $wR_2 = 0.0641$
R indices (all data)	$R_1 = 0.0203$ $wR_2 = 0.0402$	$R_1 = 0.0269$ $wR_2 = 0.0585$	$R_1 = 0.0312$ $wR_2 = 0.0665$

Gap energies calculations

The fundamental band gap energy ‘ E_g ’ and the type of transition for crystalline materials are calculated via the absorption coefficient as a function of ‘ $h\nu$ ’ near the fundamental absorption edge using the expression ¹:

$$(\alpha h\nu)^{\frac{1}{m}} = A_1 (h\nu - E_g) \quad (1)$$

“ A_1 ” and “ h ” are a constant and the Planck's constant, respectively. “ m ” is equal to 1/2 for a direct allowed transition type and 2 for an indirect allowed transition. As $F(R) \propto \alpha$, eq(3) is expressed as:

$$(F(R) \times h\nu)^{\frac{1}{m}} = A_2 (h\nu - E_g) \quad (2)$$

Taking a logarithm onto both sides and differentiating the equation (2) with respect to ‘ $h\nu$ ’, we get the following form:

$$\ln[F(R)hv] = \ln(A) + m \ln(hv - E_g) \quad (3)$$

$$\frac{d[\ln(F(R)hv)]}{d(hv)} = \frac{m}{hv - E_g} \quad (4)$$

The value of E_g is obtained from the fitted plot of $d[\ln(F(R)hv)]/d(hv)$ vs hv . The line discontinuity reveals the information about optical transitions. These are indicated at a particular maximum energy value where a particular transition might have taken place corresponding to a specific value of 'm'. The graph between $[\ln(F(R)hv)]$ and $[\ln(hv - E_g)]$ was plotted to obtain the value of 'm' which presents the slope of the linear part.

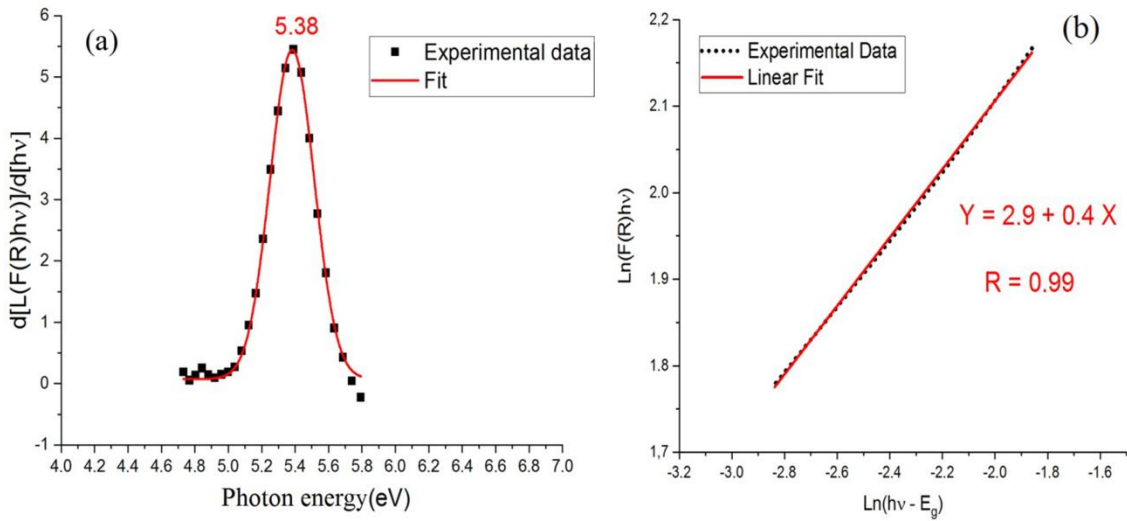


Figure S1. (a): $d[\ln(F(R)hv)]/d(hv)$ vs hv and (b): $[\ln(F(R)hv)]$ vs $[\ln(hv - E_g)]$ of the pure DMACdCl₃.

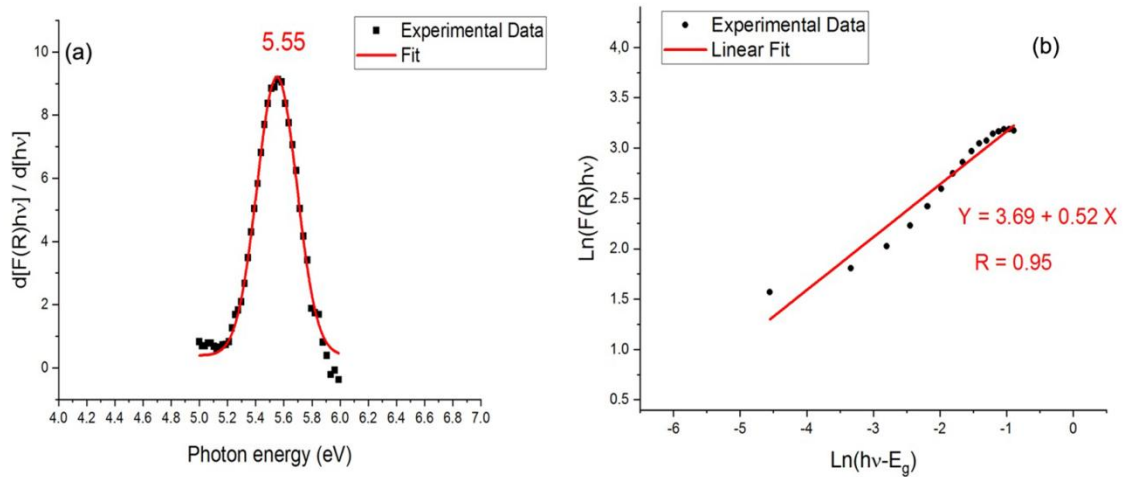


Figure S2. (a): $d[\ln (F(R)hv)]/d(hv)$ vs hv and (b): $[\ln (F(R)hv)]$ vs $[\ln (hv - E_g)]$ of the DMACdCl₃ : Zn.

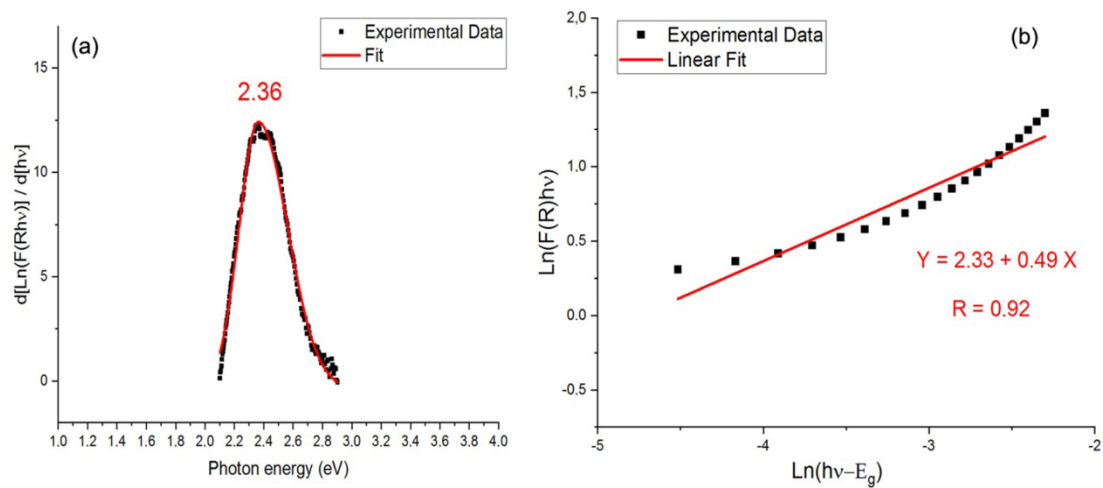


Figure S3. (a): $d[\ln (F(R)hv)]/d(hv)$ vs hv and (b): $[\ln (F(R)hv)]$ vs $[\ln (hv - E_g)]$ of the DMACdCl₃ : Cu

Reference

- 1 M. Duvenhage, M. Ntwaeaborwa, H. G. Visser, P. J. Swarts, J. C. Swarts and H. C. Swart, *Opt. Mater. (Amst.)*, 2015, **42**, 193–198.