Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Growth Methods' Effect on the Physical Characteristics of $CsPbBr_3$ Single Crystal

Mohamed Ben Bechir, [*, a] and Faisal Alresheedi [b]

[a] *Laboratory of Spectroscopic and Optical Characterization of Materials (LaSCOM), Faculty of Sciences, University of Sfax, BP1171 – 3000 Sfax, Tunisia.*

[a] *Department of Physics, College of Science, Qassim University, Buraidah 51452, Saudi Arabia.*

[*] *Corresponding author. E-mail address:* mohamedbenbechir@hotmail.com

Supplementary Figures

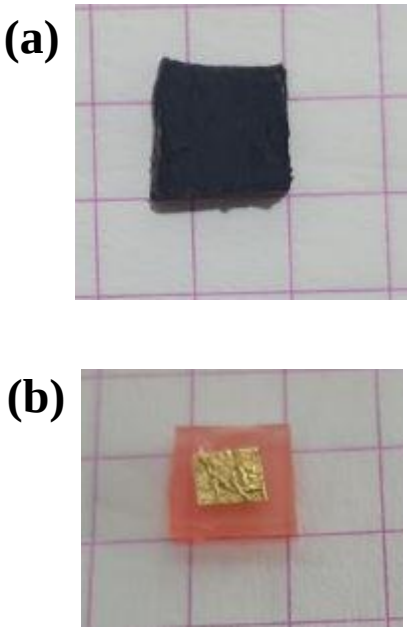

Figure. S1. Electrode Configurations for Characterizing $CsPbBr_3$ SCs: (a) Conventional SCLC and Photodetector Assessments with Carbon Electrodes, and (b) TM-SCLC Measurements with Gold Electrodes.

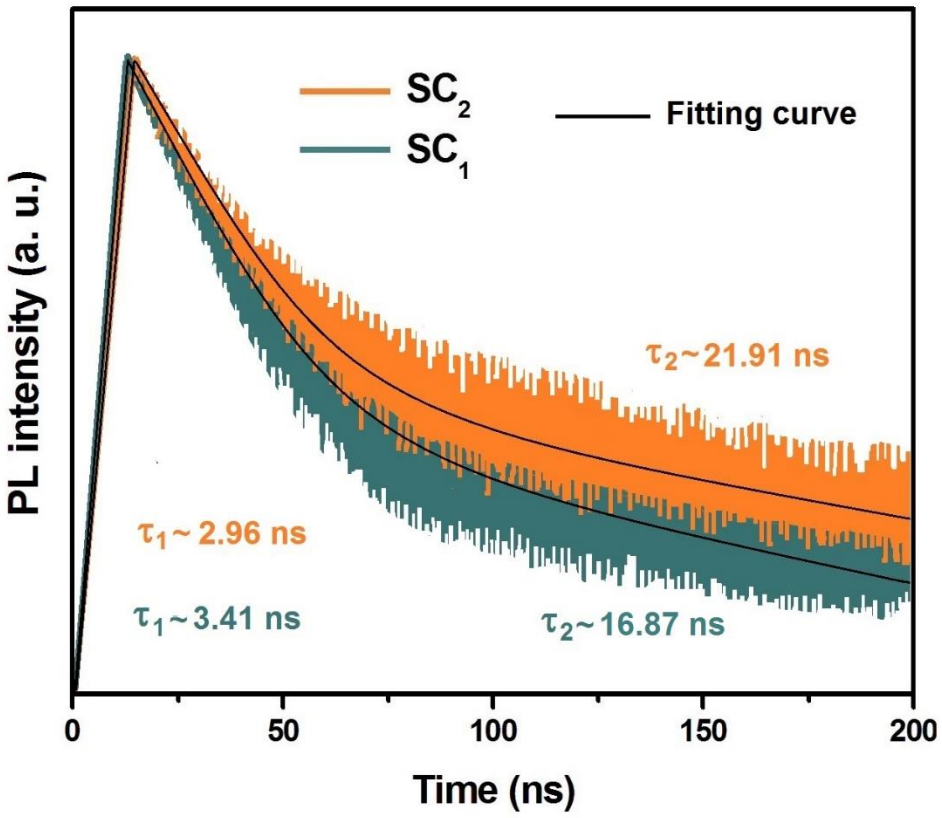

Figure. S2. Time-Resolved Photoluminescence Spectroscopy of both Crystals at room temperature.

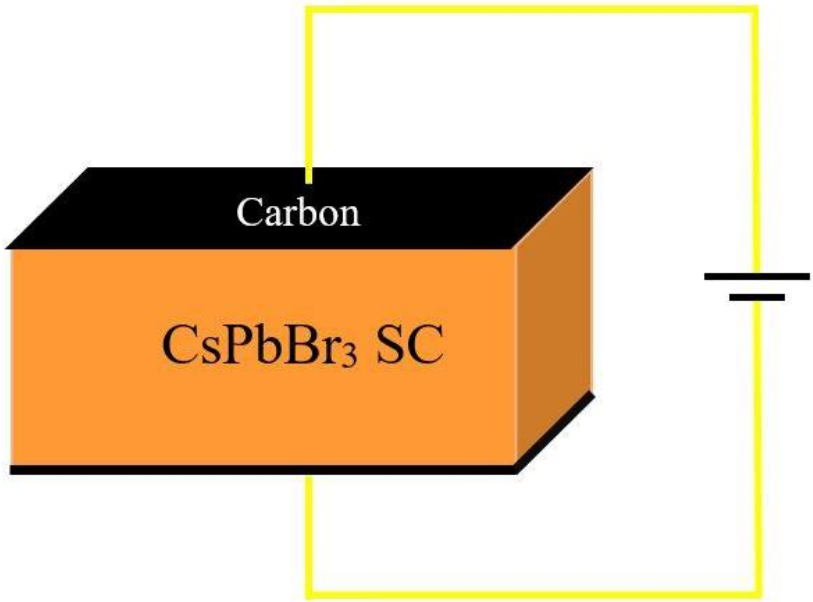

Figure. S3. Schematic Representation of Device Configuration.

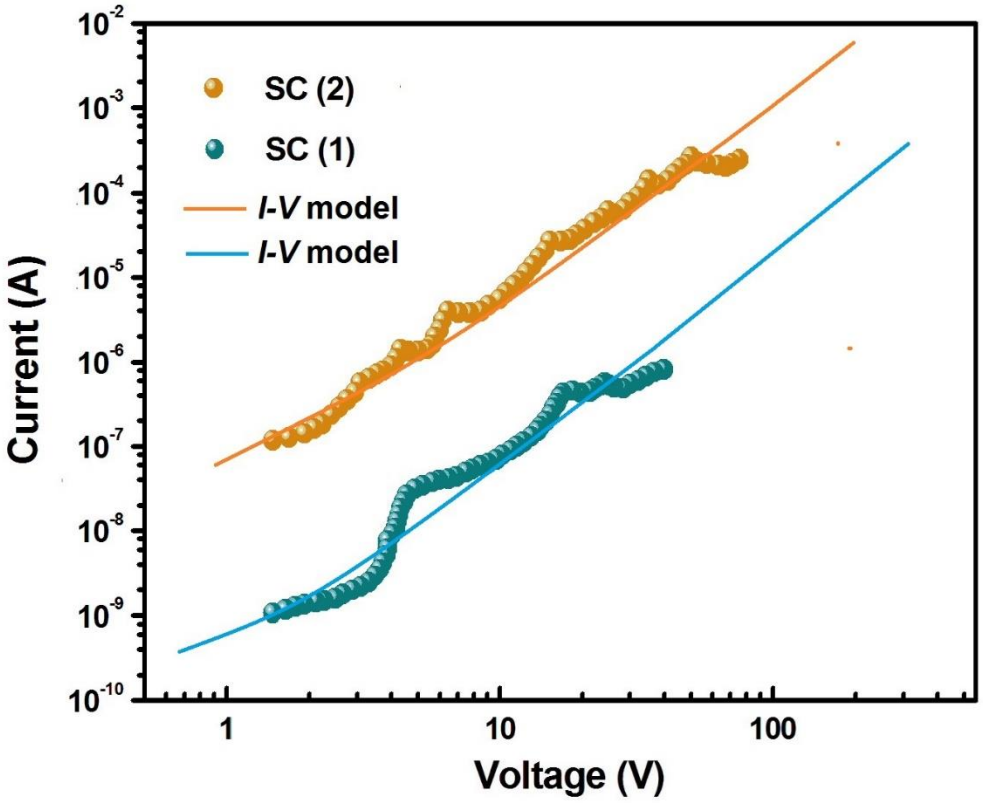

Figure. S4. Spectral Analysis of TM-SCLC Behavior for both types of $CsPbBr_3$ SCs at T = 310.15 K. Utilizing Solid Lines to Depict an I-V Model Involving Monoenergetic Transport Band and Trap for Analyzing Charge Carrier Concentrations in the Investigated Perovskite.

Supplementary Tables

Table S1. FWHM and L_s Values According to all XRD Reflections.

	FWHM (°)		L_s (%)	
Miller indices (hkl)	SC_1	SC_2	SC_1	SC_2
(020)	0.051	0.063	0.063	0.120
(101)	0.039	0.048	0.044	0.095
(040)	0.085	0.096	0.112	0.179
(202)	0.091	0.103	0.127	0.184
(060)	0.032	0.042	0.028	0.041
(303)	0.021	0.033	0.023	0.037

Table S2. Exploring Optoelectronic Characteristics via TM-SCLC in both types of $CsPbBr_3$ SCs.

	SC_1	SC_2
μ_0 ($m^2\ V^{-1}\ s^{-1}$)	0.017	0.396
n_f (cm^{-3})	2.62×10^8	2.54×10^8
n_t (cm^{-3})	8.81×10^9	2.08×10^{10}
$E_F - E_v$ (eV)	0.57	0.57
$E_t - E_v$ (eV)	0.695	0.717
$E_t - E_F$ (eV)	0.125	0.147

Supplementary Equations

$$L_s = \frac{B_s}{4\tan\theta} \tag{S1}$$

B_s characterizes structural expansion, signifying the variance in the integral profile width when comparing a standard (referred to as 'std') with the target sample slated for analysis ('obs').

$$B_{struct} = \sqrt{B_{obs}^2 - B_{std}^2} \tag{S2}$$

B_{obs} represents the width derived from the compound undergoing analysis, whereas B_{std} signifies the width derived from the standard compound, which remains unaffected by any structural broadening phenomena.

$$R = \frac{I_{ph} - I_D}{P_{irra} S} \tag{S3}$$

where I_d and I_{ph} indicated the dark current and the photocurrent, respectively. S and P_{irra} indicating the crystal surface area and the incident light intensity power, respectively.

$$D^* = \frac{R}{(2eI_D)^{1/2}} \tag{S4}$$

$$\mathrm{D} = \mathrm{D}_0 \mathrm{e}^{\left(-\frac{\Delta \mathrm{H}}{\mathrm{RT}}\right)} \tag{S5}$$

Where D represents the rate of diffusion, ΔH denotes the activation energy for diffusion, D_0 stands for the constant of diffusion, T corresponds to the temperature of the solution, and R signifies the universal gas constant.

$$n_{trap} = \frac{2\varepsilon\varepsilon_0 V_{TFL}}{eL^2} \quad \text{(S6)}$$

Incorporating essential parameters, the equation includes ε_0 (8.85×10^{-12} F/m), which denotes vacuum permittivity, ε is the dielectric constant of $CsPbBr_3$ (ε = 22), e symbolizing the elementary charge of an electron (1.6×10^{-19} C), and L standing for the thickness of the SC (2 mm).

$$\mu_d = \mu_0 \ominus = \frac{jL^3}{\varepsilon_0\varepsilon_r(1-\gamma)(2-\gamma)^2V^2} \quad \text{(S7)}$$

where μ_0 stands for microscopic mobility. The variable 'm' ($m = \frac{1}{\gamma} = \frac{d\ lnj}{d\ ln\ V}$) corresponds to the gradient of the I−V plot (refer to Figure S4(b)), while the variable Θ is characterized as $\Theta = \frac{n_f}{n_f+n_t}$, with n_t and n_f indicating the concentration of trapped charge carriers and free charge carriers, respectively.

$$n_f = \frac{L_j}{e\mu_{0(2-\gamma)V}} \quad \text{(S8)}$$

$$n_t = \frac{\varepsilon_0\varepsilon_r(1-\gamma)(2-\gamma)V}{eL^2} \quad \text{(S9)}$$

$$E_F - E_v = \frac{k_BT}{e} ln\left(\frac{n_f}{N_v}\right) \quad \text{(S10)}$$

$$E_F - E_t = \frac{k_BT}{e} ln\left(\frac{n_t}{N_t}\right) \quad \text{(S11)}$$

where k_B is Boltzmann's constant, h is Planck's constant, E_v is the energy of the valence band, N_t and N_v indicating the density of electronic states and the density of states in the valence band, respectively.