

SI updated: 29 July 2024

Supplementary Information

Perovskite Single Crystal SCLC Measurements Prediction Using Machine Learning Model

Sarvani Jowhar Khanam,^a Harinath Kuruva,^b Salman Abdul Moiz*^b and Murali Banavoth*^a

^a *Solar Cells and Photonics Research Laboratory, School of Chemistry, University of Hyderabad, Hyderabad 500046, Telangana, India.*

^b *School of Computer & Information Sciences, University of Hyderabad, Hyderabad 500046, Telangana, India*

corresponding author: E-mail: salman@uohyd.ac.in

SCLC measurements:

We have calculated the Resistivity and Conductivity of devices by applying Ohm's Law (eq. 1) to I-V curves, which has been measured using the solar simulator and Keithley 2400.

$V = IR$(1) Resistance has been calculated by fitting the I-V curve of SCLC data, following the steps below.

$$R = \frac{V}{I}$$

Dividing the area (A) in the above equation.

$$\frac{IR}{A} = \frac{V}{A}$$

$$JR = \frac{V}{A}$$

$$\log J + \log R = \log V - \log A$$

$$\log J = \log V - \log A - \log R \quad \log J = \log V - (\log A + \log R) \quad \dots\dots\dots (2)$$

Which is in the form of

$y = mx + c$ Resistance (R) has been calculated by considering the intercept of $\log J$ vs $\log V$ of SCLC data. Subsequently, compared both equations and calculated the R-value followed by resistivity (ρ) by adding resulted R values in the below equation.

$$R = \rho \frac{d}{A}$$

$$\rho = R \frac{A}{d} \dots\dots\dots(3)$$

d is the thickness of the device, ρ is resistivity, and A is the area.

Conductivity (σ) is the reciprocal of resistivity (ρ).

$$\sigma = \frac{1}{\rho} \dots\dots\dots(4)$$