

# Unraveling the Role of Traps in Understanding the Superlinear Power Law and Vacancy-Assisted Ion Conduction in Hybrid Organic-Inorganic Metal Halide Perovskite

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## Abstract

In cutting-edge energy research, organic-inorganic metal halide perovskites (OIMHPs) are at the forefront. Therefore, understanding how standard operating conditions, such as air temperature, humidity, light exposure, *etc.*, affect the transport in OIMHP-based energy harvesting devices is crucial. Here, we have examined the temperature-dependent complex impedance, complex electric modulus, and AC conductivity spectra of an OIMHP, FAPbBr<sub>2</sub>I. We have used theoretical models, such as the Havriliak Nigami model and the Jonscher Power law, to fit the obtained results. The Maxwell-Wagner equivalent circuit model has been utilized to decipher the resistive and capacitive contributions of grains and grain boundaries to the total impedance at various temperatures. The AC conductivity spectra exhibit distinct behaviors in two different temperature zones, viz. at low-temperature (LT) and high-temperature (HT) zones. Normal ionic conduction with sublinear dispersion was discovered in the LT region (323-403 K) where the frequency exponent ( $n$ ) < 1. In the HT regime (413-463 K), the sublinear dispersion transforms into a superlinear dispersion ( $n$ ) > 1. The appearance of a superlinear (SPL) AC conductivity dispersion beyond a critical temperature of 413 K is ascribed to the decoupling or the release of a large number of charge carriers from the trap centers in the HT regime. Additionally, we notice an immediate increase in DC conductivity beyond 413 K, which can be attributed to the dominance of vacancy-assisted ionic conduction because, when the charge carriers are discharged, the vacancies constituting the trap states become accessible for ionic conduction. Moreover, by investigating the temperature-dependent space charge limited current-voltage characteristics of FAPbBr<sub>2</sub>I single crystal, we have unveiled the role of trap states in understanding the SPL behavior and vacancy-mediated ionic conduction. Finally, it is noted that although the complex electric modulus and AC conductivity scale to a master curve in the LT regime, the scaling leads to the non-overlapping curves in the dispersive high-frequency region of the HT regime, further supporting the existence of two distinct dispersion behaviors and conduction mechanisms in the low- and high-temperature regimes.

## Keywords

Single Crystal, Superlinear Power Law, Ionic Conduction, Space Charge Limited Current, Dielectric Relaxation, Conductivity Scaling