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Supplementary information to:

Polaron Transport in Hybrid $CH_3NH_3PbI_3$ Perovskite thin films

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In order to investigate transport mechanisms in a prototypical $CH_3NH_3PbI_3$ thin film, we considered the charge-carrier scattering due to lattice defects and LO phonon. In numerical calculations, we used the constant parameters in Table S1 to fit carrier mobility data measured by TRTS techniques (sum of both electron and hole mobilities) for the $MAPbI_3$ thin film [1]. The first process is an ionized impurity (II) scattering. The MA interstitials (I_{MA}) and Pb vacancies (V_{Pb}) [2,3], were monitored as the scattering center. A standard approach [4], Brooks-Herring formula, was used to describe the scattering of ionized impurities as:

$$\mu_{II} = \frac{128\sqrt{2\pi}(\varepsilon_0\varepsilon_s)^2(k_BT)^{3/2}}{\sqrt{m^*}Z^2e^3N_I[\ln(1+\beta)-\beta/(1+\beta)]}, \quad \text{(S1)}$$

where $\beta = 24\varepsilon_0\varepsilon_s m^*(k_BT)^2/\hbar^2e^2n$, n is the density of charge-carrier, N_I is the density of an ionized impurity, and Z is the ionic charge of an ionized impurity. The second process is polaron-LO phonon scattering. The LP polaron mobility formula, Eq. (2) in the main text, was adopted to calculate the mobility.

In order to predict charge-carrier mobility in the orthorhombic phase, the effective masses of the electron and hole as well as dielectric functions related the structural phase transition in Table S1, were applied in the calculations. We used Matthiessen's rule based on $\mu_{tot}^{-1} = \sum_i \mu_i^{-1}$ to determine the total charge-carrier mobility. This rule assumes that various scatterings operate independently of each other. If one scattering mechanism dominates, other scatterings can be ignored. Figure S1 shows the fitted mobilities and experimental data [1] in the orthorhombic phase. The total charge-carrier mobility, $\mu_{tot}^{-1} = \mu_{II(I_{MA})}^{-1} + \mu_{II(V_{Pb})}^{-1} + \mu_{LO}^{-1}$, was in very good agreement with the experimental data over the whole temperature range. The fitting result suggested that the scattering from ionized impurities is predominant at $T < 80$ K.

Table S1. The constant parameters used in the calculation

Parameter	Symbol (units)	Value
$MAPbI_3$ perovskite		
Effective masses	m_e^* (kg)	$0.23m_0$ [5] (orthorhombic phase)
	m_h^* (kg)	$0.39m_0$ [5] (orthorhombic phase)
LO phonon energy	$\hbar\omega_{LO}$(meV)	11.5 [6]
Charge-carrier densities	$n = n_e = n_h$ (cm^{-2})	5×10^{14}
Density of MA interstitial	$N_{I_{MA}}$(cm^{-3})	2×10^{16}
Density of Pb vacancy	$N_{V_{Pb}}$(cm^{-3})	2×10^{16}
Ionic charge of MA interstitial	Z	+1.0
Ionic charge of Pb vacancy	Z	+2.0

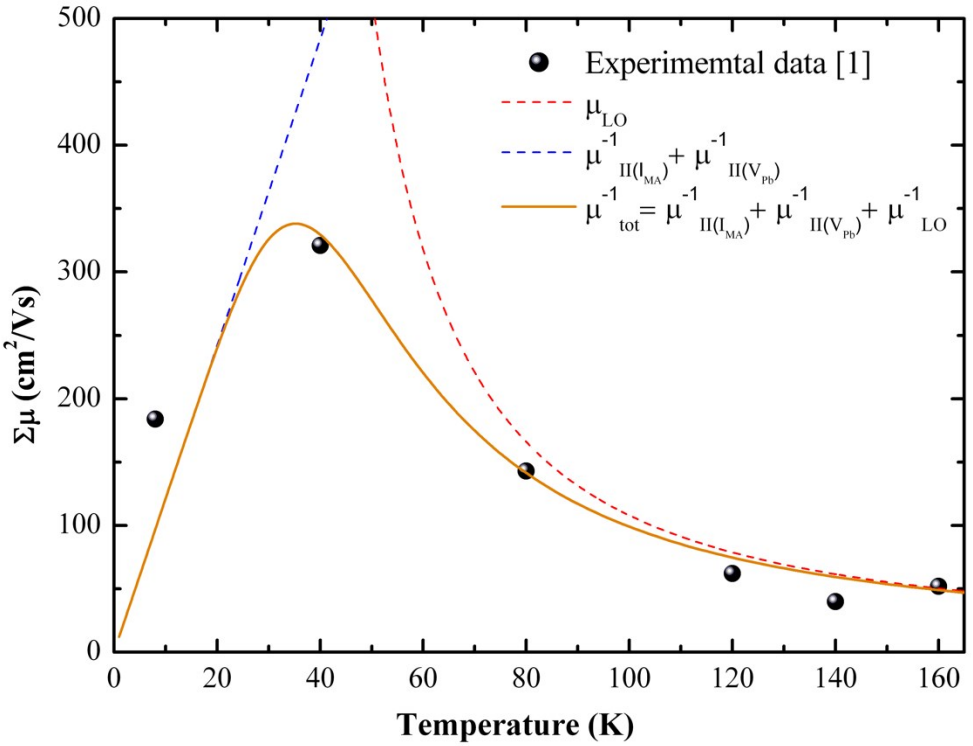

Figure S1: Temperature dependence of the fitted mobilities and the experimental results [1]. The dashed lines represent the individual scattering limited mobilities. The solid line represents the total mobility.

Supplementary references

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