The Efficiency Limit of $CH_3NH_3PbI_3$ Perovskite Solar Cells

Wei E.I. Sha[1,2], Xingang Ren[1], Luzhou Chen[1], and Wallace C.H. Choy[1, a)]

1. *Department of Electrical and Electronic Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, China*
2. *The University of Hong Kong Shenzhen Institute of Research and Innovation (HKU-SIRI), Shenzhen, 518057, China.*

[a)]Electronic mail: chchoy@eee.hku.hk

Supplementary Material

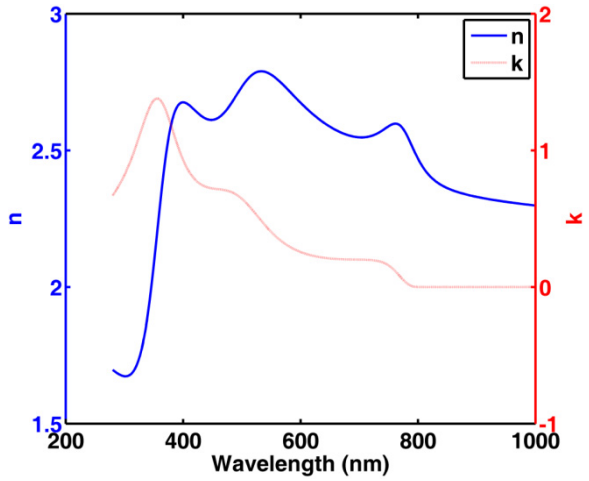

FIG. S1. Complex refractive index of $CH_3NH_3PbI_3$ perovskite materials.

Nonradiative Recombination Incorporated Detailed Balance Model

To analyze the influence of trap-assisted nonradiative recombination on the efficiency limit of $CH_3NH_3PbI_3$ solar cells, the detailed balance model should be modified as

$$J(V) = J_t(V) + J_e(V) - J_p \tag{S1}$$

where V is the applied voltage of the solar cell system. J_p is the photocurrent (photogenerated current) due to absorption of incident sunlight. J_e and J_t describe current density losses due to the radiative emission and trap-assisted nonradiative recombination, respectively. For perovskite solar cells, the dominant nonradiative recombination process is the monomolecular (or Shockley-Read-Hall) recombination. Therefore, the nonradiative current can be expressed as

$$J_t(V) = q\gamma n_i W \exp\left(\frac{0.5qV}{k_B T}\right) \tag{S2}$$

where γ is the monomolecular (recombination) rate, n_i is the intrinsic carrier density, and W is the cell thickness. q is the elementary charge, k_B is the Boltzmann constant, and T is the kelvin temperature.

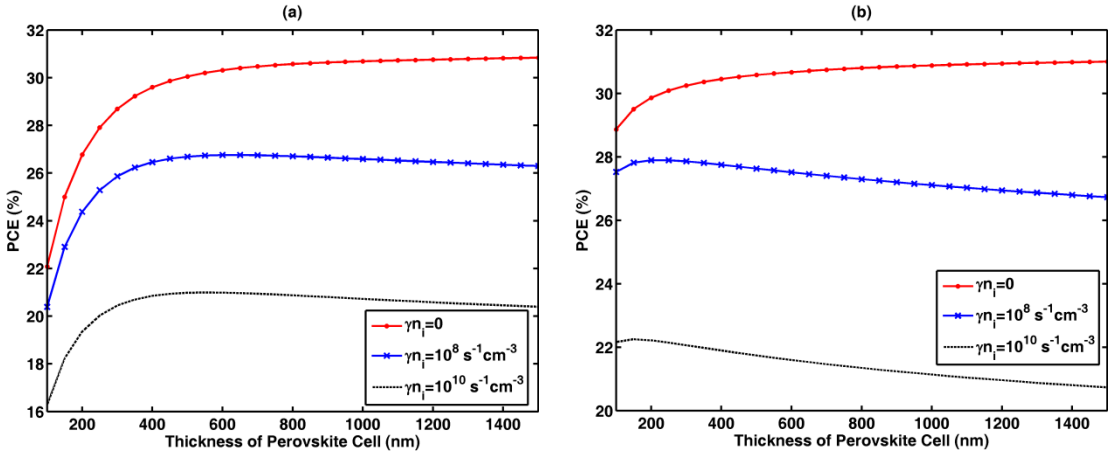

FIG. S2. Nonradiative-recombination dependent device efficiency of perovskite solar cells (without angular-restriction designs). The nonradiative recombination is proportional to the product of the monomolecular (recombination) rate γ and intrinsic carrier density n_i. (a) flat cell with a perfectly reflecting mirror; (b) textured

cell with a perfectly reflecting mirror. For achieving the best device efficiency, the active-layer thickness of textured cells is much smaller than that of flat cells.

Figure S2 shows nonradiative-recombination dependent device efficiency of perovskite solar cells. For both flat and textured cells, nonradiative recombination degrades the device efficiency significantly. An optimized thickness of active layer should be carefully selected for different light-trapping designs. For example, the active-layer thickness of textured cells should be smaller than 200 nm for achieving the best efficiency. **Figure S3** depicts the influence of nonradiative recombination on the angular-restriction designs. For flat cells, no improvements can be found even if we have adopted the wavelength-dependent angular restrictions. In view of a very weak optical absorption at long wavelengths, the radiative current of flat perovskite cells is quite small compared to the nonradiative (recombination) current, particularly under the maximum power point and open-circuit voltage conditions. This feature is critically different from GaAs materials with a stronger optical absorption at long wavelengths. Thus, the radiative and nonradiative currents of GaAs solar cells have comparable amplitudes. In contrast to flat perovskite cells, the device efficiency of textured perovskite cells still can be improved due to enhanced absorptivity as presented in Eq. (4) of manuscript.

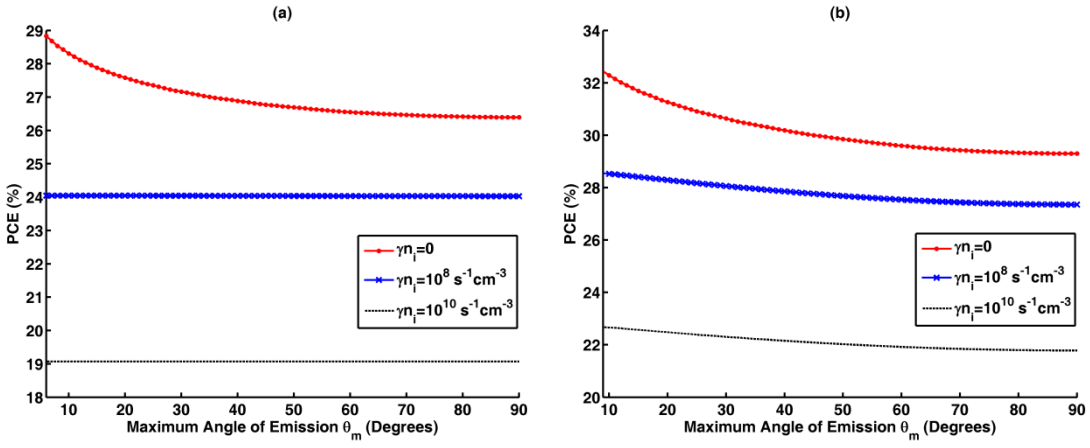

Figure S3. Device efficiency of perovskite solar cells as a function of maximum emission angle. The influence of nonradiative recombination on angular-restriction designs is investigated. The nonradiative recombination is proportional to the product of the monomolecular (recombination) rate γ and intrinsic carrier density n_i. A wavelength-dependent angular-restriction design is adopted, i.e. an angular-restriction filter is applied only to the wavelength range of 700 nm to 1000 nm. At the wavelengths with (without) the angular-restriction filtering, the direct AM 1.5D (global AM 1.5G) spectrum of Sun is used in the calculations. (a) flat cell with a perfectly reflecting mirror; (b) textured cell with a perfectly reflecting mirror. In contrast to flat cells where no improvement can be found, the wavelength-dependent angular-restriction design increases the power conversion efficiency of textured cells by improving absorptivity [See Eq. (4) in manuscript].