Area: Perovskite Solar Cells

VARIATION OF OPTICAL ABSORPTION WITH CENTER CATION IN HYBRID PEROVSKITE SOLAR CELLS

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Hybrid perovskite solar cells have received great attention due to high conversion efficiencies exceeding 20% and possible low-cost fabrication of the modules. It has been reported that, when a HC(NH₂)₂PbI₃ (FAPbI₃) hybrid perovskite is mixed with CH₃NH₃PbI₃ (MAPbI₃), the conversion efficiency improves due to the reduction of the band gap. In this study, we have performed the spectroscopic ellipsometry (SE) analyses of the FAPbI₃ and EQE simulation of a FAPbI₃ solar cell particularly to reveal the absorption characteristics of FAPbI₃. Furthermore, the effect of the center cation in APbI₃-type hybrid perovskites on the absorption properties has been investigated based on density functional theory (DFT) analysis.

The FAPbI₃ layers were fabricated by laser evaporation technique [1]. The SE measurements of the FAPbI₃ layers were performed in a N₂ ambient without exposing the samples to air [2]. Figure 1 shows the absorption coefficient (α) spectra of FAPbI₃ and of MAPbI₃, which were reported in our previous study [3]. Open circles and solid lines in Figure 1 indicate experimental and DFT calculation results, respectively. As shown in Figure 1, the α values of FAPbI₃ are notably lower than those of MAPbI₃, and the α spectrum changes rather significantly by the change of the center cation. The α spectra calculated from DFT reproduce the experimental spectra well, supporting the validity of our analysis. Detailed DFT analysis reveals that the difference of α between MAPbI₃ and FAPbI₃ is caused by the strong interaction of the I-N atoms induced by the hydrogen bonding (i.e., I···H-N) [2]. Figure 2 shows the experimental EQE spectrum of the FAPbI₃ solar cell (open circles) reported in Ref. [4], together with the calculation result obtained from the EQE simulation (solid line) [2]. The EQE simulation was preformed using the optical model indicated in the inset based on the procedure established in our study [3]. The calculated EQE spectrum shows the good agreement with the experimental spectrum, although the band-gap region shows slight difference. From the above results, we further discuss the optical transition in hybrid perovskite solar cells.


Figure 1: α spectra of HC(NH₂)₂PbI₃ and CH₃NH₃PbI₃ obtained from spectroscopic ellipsometry and DFT calculation.

Figure 2: EQE spectral of the HC(NH₂)₂PbI₃ solar cell. The experimental data are adopted from Ref. [4].