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 $HC(NH_2)_2PbI_3$ ($FAPbI_3$) hybrid perovskite is mixed with $CH_3NH_3PbI_3$ ($MAPbI_3$), 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 $FAPbI_3$ and EQE simulation of a $FAPbI_3$ solar cell particularly to reveal the absorption characteristics of $FAPbI_3$. Furthermore, the effect of the center cation in $APbI_3$-type hybrid perovskites on the absorption properties has been investigated based on density functional theory (DFT) analysis.

The $FAPbI_3$ layers were fabricated by laser evaporation technique [1]. The SE measurements of the $FAPbI_3$ layers were performed in a N_2 ambient without exposing the samples to air [2]. Figure 1 shows the absorption coefficient (α) spectra of $FAPbI_3$ and of $MAPbI_3$, 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 $FAPbI_3$ are notably lower than those of $MAPbI_3$, 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 $MAPbI_3$ and $FAPbI_3$ 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 $FAPbI_3$ 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.

[1] Miyadera et al., ACS Appl. Mater. Interfaces **8**, 26013 (2016), [2] Kato et al., J. Appl. Phys. **121**, 115501 (2017), [3] Shirayama et al., Phys. Rev. Applied **5**, 014012 (2016), [4] Yang et al., Science **348**, 1234 (2015).

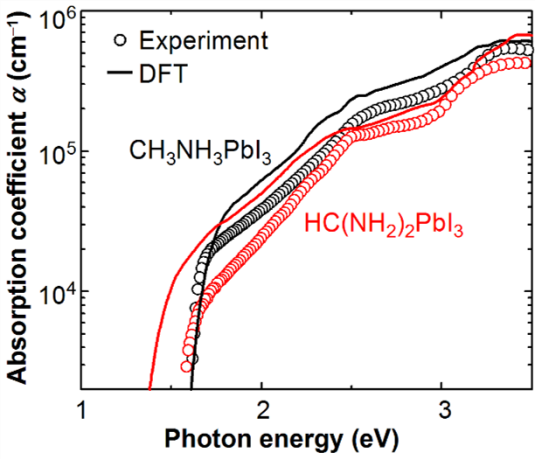

Figure 1: α spectra of $HC(NH_2)_2PbI_3$ and $CH_3NH_3PbI_3$ obtained from spectroscopic ellipsometry and DFT calculation.

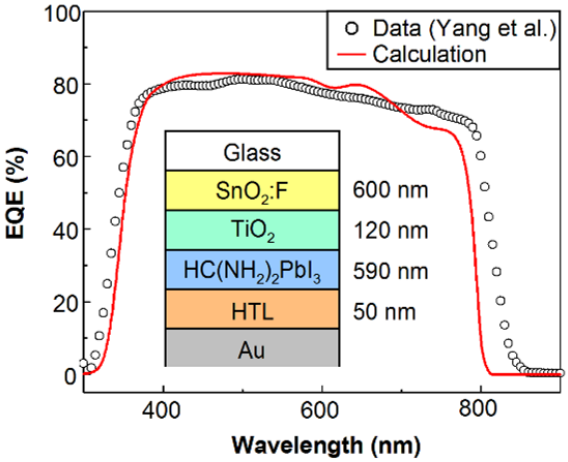

Figure 2: EQE spectral of the $HC(NH_2)_2PbI_3$ solar cell. The experimental data are adopted from Ref. [4].