ドナーアクセプター型共重合体をホール輸送層として用いたペロブスカイト太陽電池におけるパッシベーションの効果

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Background & Motivation

Background

・The power conversion efficiency (PCE) of perovskite solar cells (PSCs) has risen up to 25.2%.

・HTMs have been actively explored. The exploration mainly focused on the following three characteristics:
1) Long-term stability.
2) High hole mobility.
3) Suitable frontier energy levels matching that of perovskite layer.

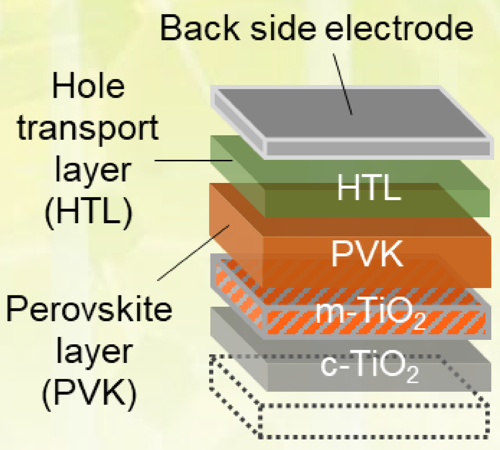


Fig. 1 Typical mesoporous-type device structure.

Spiro-OMeTAD
→ Typical HTM. Li-TFSI is added as dopant.
→ Relatively expensive.
>> Alternative materials have been explored.

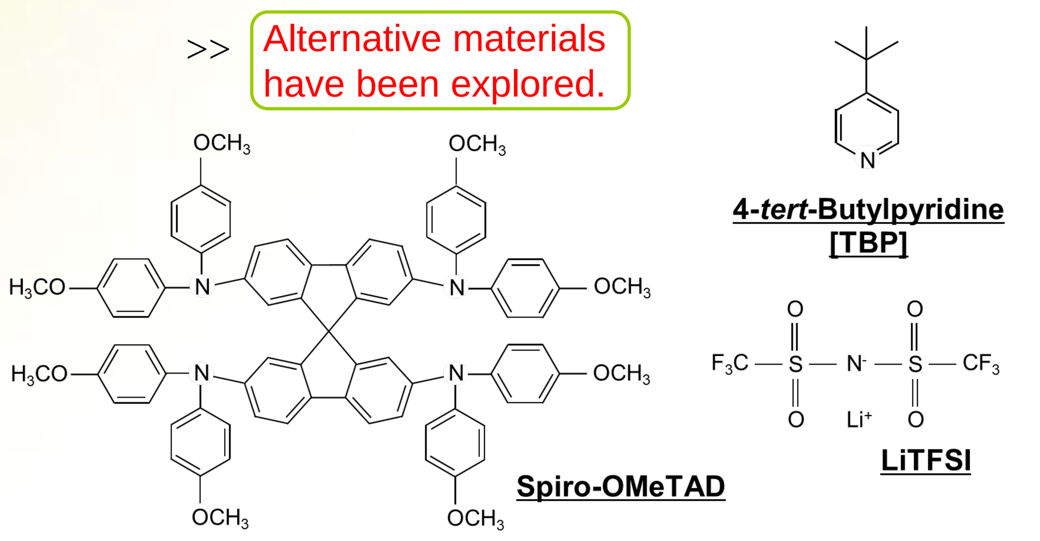


Fig. 2 Molecular structures of Spiro-OMeTAD and dopants.

Donor-acceptor (D-A) copolymer
・Simple synthetic method
・Good stability
・Flexible electron density distribution

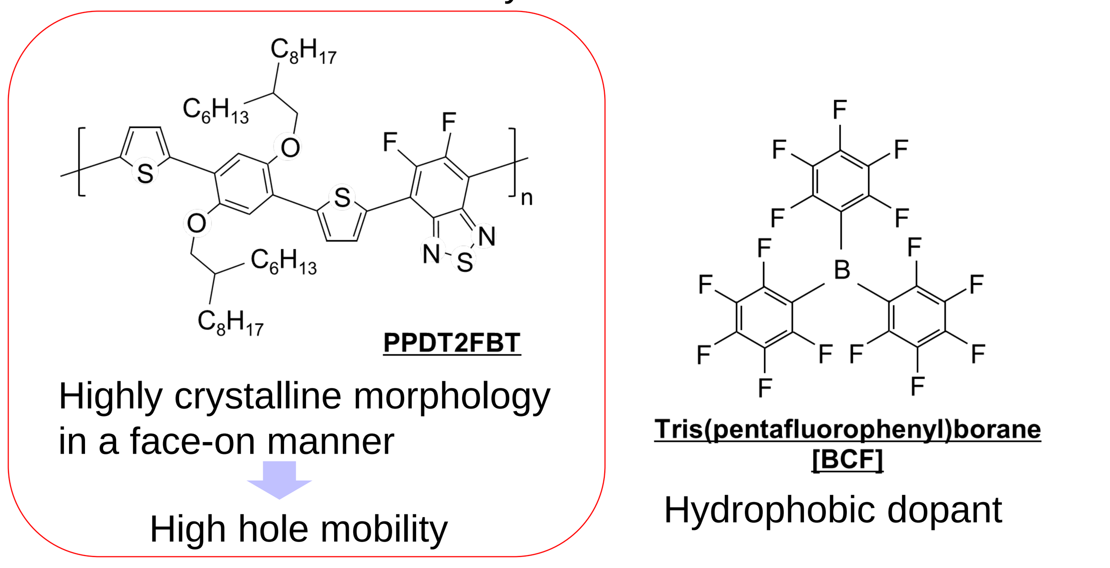


Fig. 3 Molecular structure of PPDT2FBT[1] and BCF

Experimental

Device fabrication

● Inside of glove box ●
Environment : N_2 atmosphere
O_2 < 15 ppm. H_2O < 10 ppm.

I. Compact TiO_2 layers (c-TiO_2)
・Spray pyrolysis method.

II. Mesoporous TiO_2 layers (m-TiO_2)
・Spin coating of TiO_2 particles-dispersed solution, and baking at 450°C.

III. Perovskite layers (PVK)
・PVK precursor solution.
(Solvent : DMSO+DMF)
$[Cs_{0.05}FA_{0.79}MA_{0.16}PbI_{2.52}Br_{0.48}]$
>> PVK layers formed by the anti solvent method.

IV. Hole Transporting Layers (HTL)
・HTM solution. (Solvent : truene)
[PPDT2FBT] (Preheating : 80°C)
PPDT2FBT with BCF
>> Spin coating

V. Au electrodes
・Vacuum evaporation.

Keeping in dry air

● desiccator ●
Environment : Under the dry air.
Humidity : < 5%RH
Temperature : 20 ~ 25°C
UV shielding

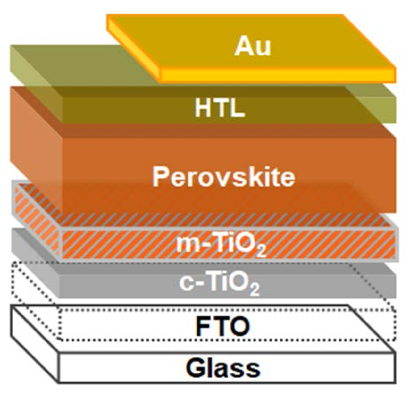
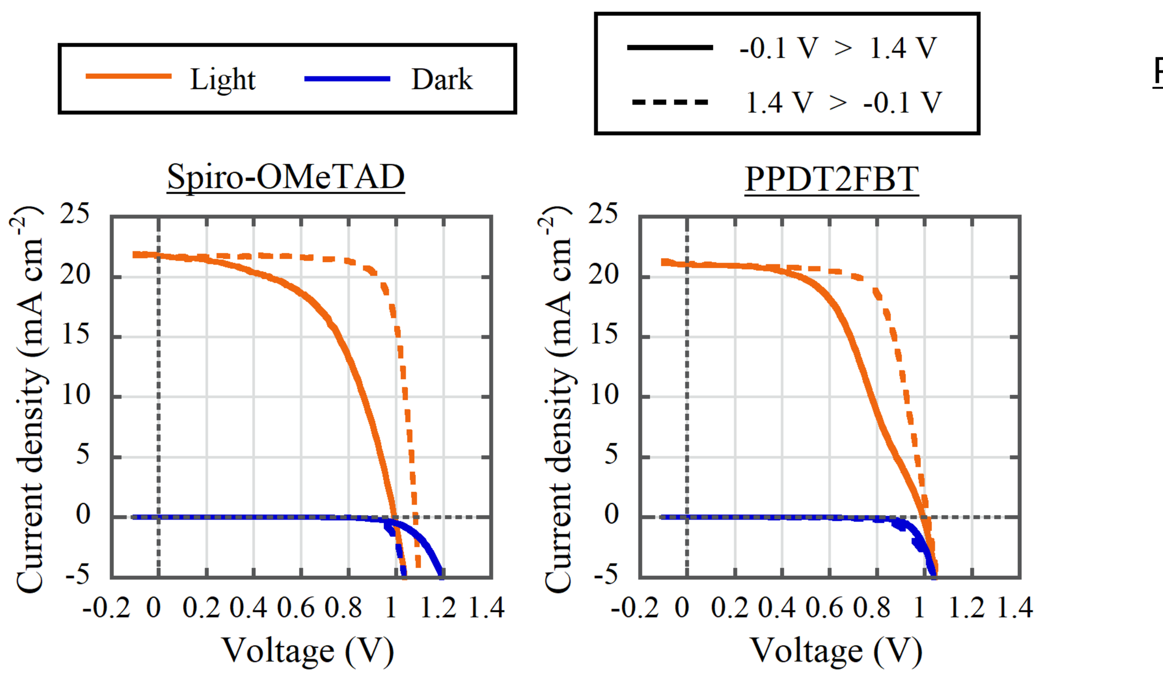


Fig. 4 Device structure.

Results and Discussion

J-V measurement



PCE : 18.52%
J_{sc} : 21.66 mA/cm², V_{oc} : 1.08 V
FF : 0.79

PCE : 14.93%
J_{sc} : 21.05 mA/cm², V_{oc} : 1.01 V
FF : 0.70

The PCE of PPDT2FBT based devices decreased compare to that of standard PSCs with spiro-OMeTAD.

Fig. 5 *J-V* characteristics of spiro-OMeTAD and PPDT2FBT based devices.

FABr passivation [2]

Passivation
・**FABr** / IPA solution [5 mg/mL]
>> spin coating
→ 100℃ / 5 min

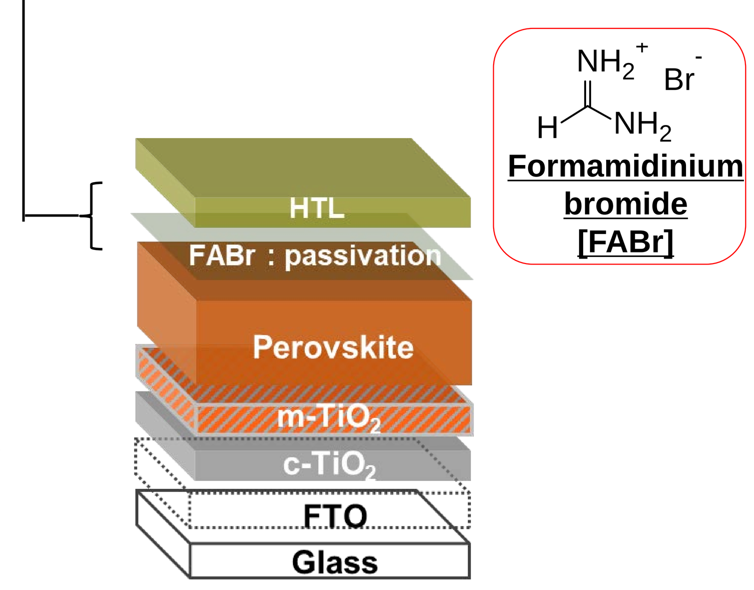


Fig. 6 Device structure with FABr passivation

XRD spectra

After FABr passivation on perovskite, the peak of PbI_2 disappeared.

→PbI_2 dose not remained.
→An additional $FAPbBr_{3-x}I_x$ was constructed.

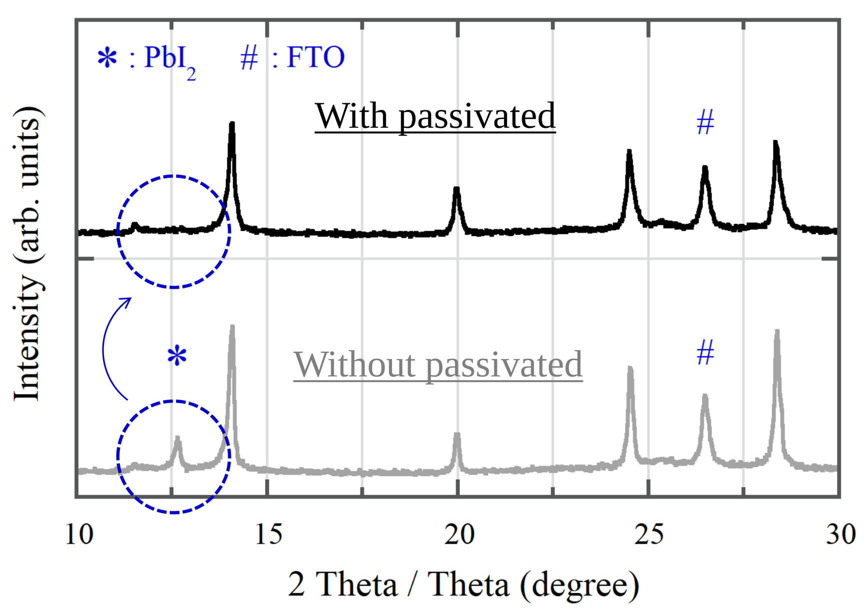
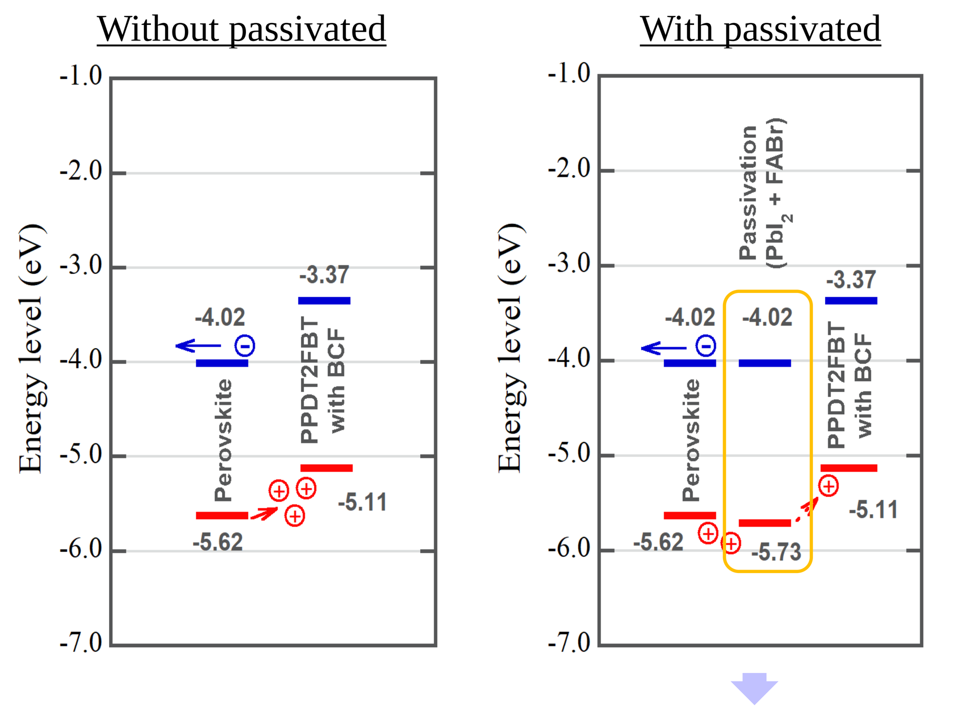


Fig. 7 XRD spectra of with or without passivation layer.

Band diagram

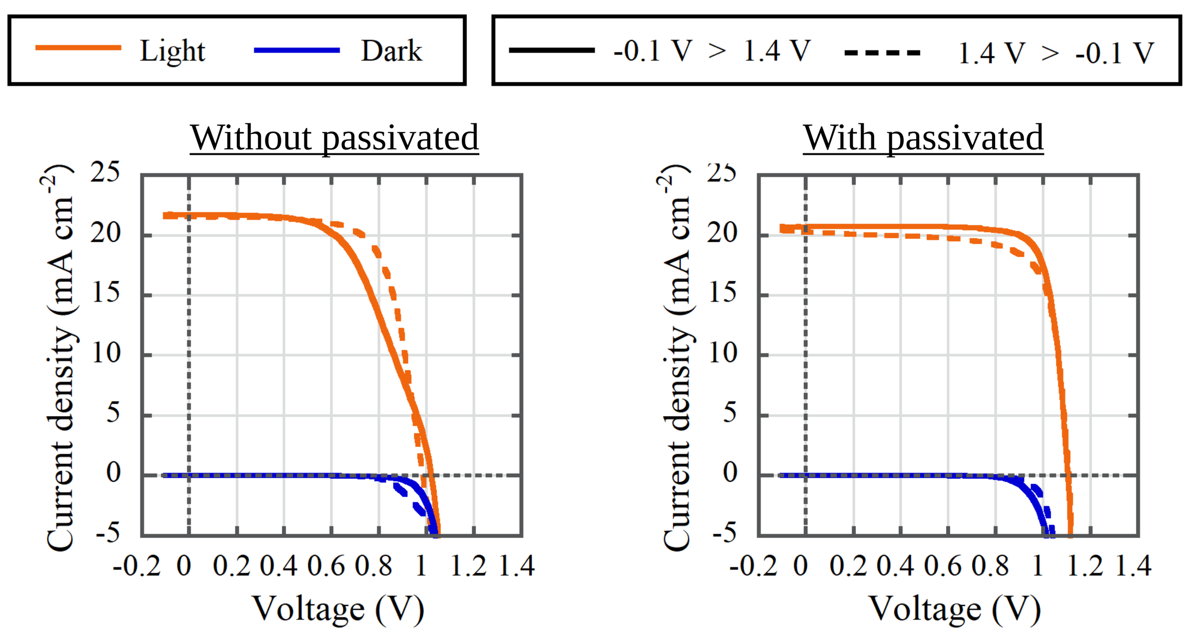
Energy levels are calculated by using PYS (photoelectron yield spectroscopy) and UV-vis spectroscopy. (The arrows indicate the recombination process of electrons.)



The carrier recombination was suppressed by inserting the passivation layer.

Fig. 8 Inferred charge recombination mechanism

J-V measurement of the optimized devices



PCE : 14.81%
J_{sc} : 21.53 mA/cm², V_{oc} : 0.98 V
FF : 0.70

PCE : 18.40%
J_{sc} : 20.69 mA/cm², V_{oc} : 1.10 V
FF : 0.81

Fig. 9 *J-V* characteristics of the optimized PPDT2FBT based devices without or with passivation layer.

Summary

・We investigated a D-A copolymer (PPDT2FBT), as a HTL in PSCs.

・It was turned out that the valence band level of FABr passivation layer was slightly lower than that of perovskite layer.

・PSCs treated with FABr solution showed higher open-circuit voltage and fill factor than those of untreated cells. This result indicates that the passivation layer prevents a backflow of holes from a HTL to the perovskite to suppress charge recombination.

・For the optimized PPDT2FBT based devices, the PCE was recorded 18.4%.

References

[1] C. W. Koh, J. H. Heo, M. A. Uddin, Y. –W. Kwon, D. H. Choi, S. H. Im, H. Y. Woo, ACS Appl. Mater. Interfaces, **9**, 43846 (2017).
[2] K. T. Cho, S. Paek, G. Grancini, C. Roldán-Carmona, P. Gao, Y. Lee, M. K. Nazeeruddin, Energy Environ. Sci., **10**, 621 (2017).

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