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Dependence of Photovoltaic Performance of Mesogenic - Phthalocyanine - Based Bulk Heterojunction Solar Cell on Alkyl Substituent Length

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はじめに：　Recently, a mesogenic phthalocyanine derivative 1,4,8,11,15,18,22,25-octaalkylphthalocyanine ($CnPcH_2$), as shown in Fig.1, has been demonstrated as a promising small molecule for use in bulk heterojunction solar cells.[1, 2] In particular, solar cells, in which the active layer was composed of $C6PcH_2$ and a fullerene derivative, 1-(3-methoxy-carbonyl)-propyl-1-1-phenyl-(6,6)C_{61} (PCBM), showed relatively high power conversion efficiency (PCE) exceeding 4.2%.[3] Although the alkyl side-chain plays one important role for packing $CnPcH_2$ molecules in hexagonal structure, the details of their effects are clarified. Herein, we report the dependence of photovoltaic performance of the solar cells on alkyl substituent length of $CnPcH_2$.

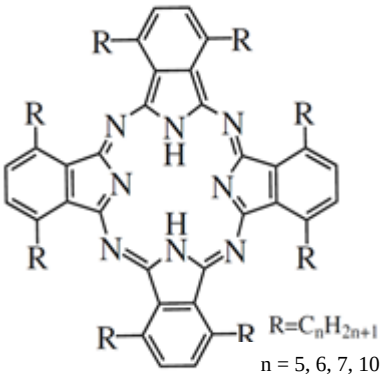

Fig. 1: Molecular structure of $CnPcH_2$

実験：MoO_x films were thermally evaporated onto ITO substrates. A solution containing a mixture of $CnPcH_2$:[70]PCBM (3:2) in chloroform with 1,8-diiodooctane, was spin-cast onto a MoO_x layer. Finally, a LiF buffer layer and an aluminum layer were deposited through a shadow mask by thermal evaporation.

結果：Figure 2 shows the J-V characteristics of solar cells in structure of ITO/MoOx/CnPcH2:[70]PCBM/LiF/Al. The device utilizing $C10PcH_2$ as a donor material showed a PCE of 0.22%, with a short-circuit current density (J_{sc}) of 1.23 mA/cm^2, an open-circuit voltage (V_{oc}) of 0.65 V, and a fill factor (FF) of 0.28. By reducing the length of alkyl substituents, the photovoltaic performance has been improved. By utilizing $C6PcH_2$, the J_{sc} increased to 9.63 mA/cm^2 and PCE of 3.72% has been achieved. Further, the dependence of the photovoltaic performance on the alkyl-chain length has been discussed, by taking the highest occupied molecular orbital of the $CnPcH_2$, the absorbance spectra of $CnPcH_2$ and packing of $CnPcH_2$ molecules in hexagonal structure into consideration.

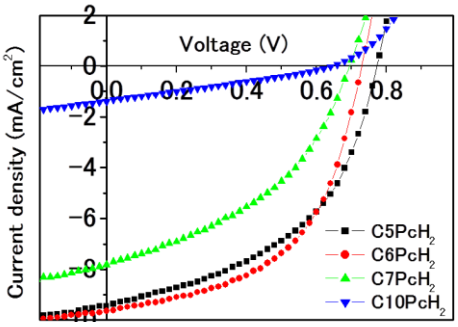

Fig. 2: J-V characteristics of solar cells

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