Regioselective fullerene-based acceptors in improved open circuit voltage for bulk-heterojunction solar cells

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Bulk-heterojunction (BHJ) solar cells based on conjugated polymer/fullerene blends showed power conversion efficiency over 3%.[1] However; it is still quite modest for practical use. Essential parameters which determine the power conversion efficiency of photovoltaic devices are the short-circuit current (J_{sc}), the open circuit voltage (V_{oc}), and the fill factor. Among them, the V_{oc} in BHJ solar cells is directly related to the first reduction potential (E^1_{red}) of the fullerenes as an electron acceptor because the electronic structure of the acceptor contributes to improvement of the open circuit potentials in a BHJ solar cell. The use of fullerene derivatives to the BHJ solar cell guarantees processability and small reorganization energy for intermolecular electron transfer. In order to increase the V_{oc}, it is required that the fullerene derivative as an acceptor has lower reduction potential than that of [6,6]-phenyl C_{61}-butyric acid methyl ester (PCBM).[3] While the tuning of the reduction potential of fullerene-based materials has also been attempted by other research groups, most studies have not succeeded in the preparation of the fullerene derivative which surpasses PCBM at first reduction potential. The regioselective multi-functionalization to fullerene core is effective to improve the electronic properties of fullerene derivative, but it was impossible to control positions of addition reaction sites.

Recently, we have developed a novel method for converting fullerene epoxides, $C_{60}O_n$, into 1,3-dioxolane compounds (scheme 1).[4] It made regioselective synthesis of fullerene derivative possible by using isolated $C_{60}O_n$ isomers. Using this method, we synthesized some fullerene-1,3-dioxolanes regioselectively to examine acceptability in the BHJ solar cell. The first reduction potentials of them obtained by differential pulse voltammetry (DPV) were compared with LUMO energy obtained from the semiempirical molecular orbital calculation (PM3). The E^1_{red} of bis-dioxolane **2b** was nearly equal to that of PCBM as shown in Table 1. In the same way, other poly-dioxolane compounds are expected to be acceptors which are superior to PCBM. These fullerene derivatives were also applied to the acceptor in BHJ solar cell devices. The details of undergoing the device characterization will be discussed at the meeting.

References

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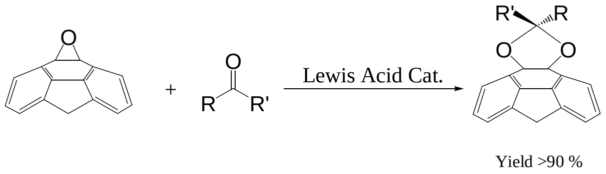
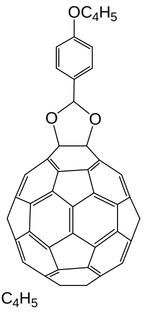
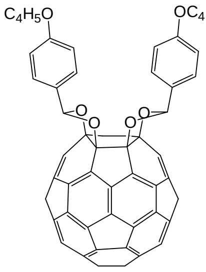


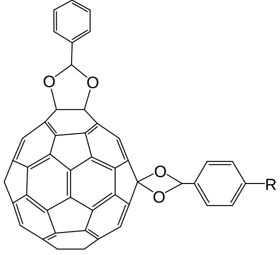
Scheme 1.



1



2a



2b

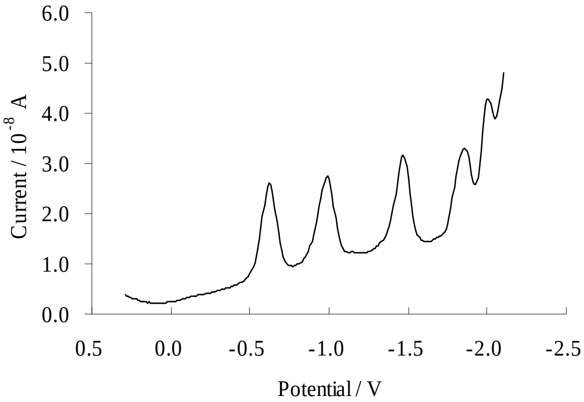


Fig. 1. DPV of **2b** at 50 mV/s scan rate, 50mV pulse, 50 ms pulse width, and 200 ms period, *o*-dichlorobenzene / 0.1 M tetrabutylammonium hexafluorophosphate as supporting electrolyte at R.T.

Table 1. Reduction peak potentials (V vs Ag/Ag$^+$) using DPV and calculated LUMO (eV) of C_{60} and fullerene derivatives.

	E^1_{red}	LUMO
C_{60}	-0.54	-2.8893
PCBM	-0.62	-2.8064
1	-0.54	-2.8745
2a	-0.52	-2.8337
2b	-0.62	-2.7751