Electrochemical characterization of polymer electron donors for organic solar cells

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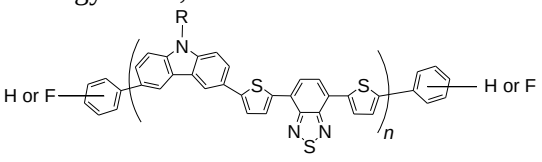
Development of novel polymer compounds is essential to the fabrication of efficient and durable organic photovoltaics (OPVs). Suitable materials can be developed, tailoring the HOMO and LUMO levels of the compounds. In this report, cyclic voltammetry was used for the determination of HOMO and LUMO levels of two highly promising materials belonging to the PCDTBT class of alternating donor-acceptor polymers. The structures of the examined polymers are given in Scheme 1. The effect of the end-groups employed to cap the macromolecular chains (either phenyl or perfluorophenyl) and of their molecular weight on the polymers energy levels, was evaluated.



R = octyl (OC), ethylhexyl (EH)

P3,6C^{R}DTBT-(Ph or 5F)

Scheme 1: Chemical structures of the two polymers studied.

The experiments were carried out with use of an Autolab electrochemical analyzer. A three electrode cell was used, consisting of a platinum wire counter electrode, an Ag/AgCl reference electrode and an ITO/Glass working electrode versus ferrocene. The polymers were drop-casted from solution on the ITO conductive side. The HOMO and LUMO levels were calculated by the following empirical relations with use of the Fc level of -4.8 eV [1,2]:

$$E_{HOMO} = -e\left(E_{onset}^{ox} - E_{1/2}^{Fc}\right) - 4.8\,[eV], \quad E_{LUMO} = -e\left(E_{onset}^{red} - E_{1/2}^{Fc}\right) - 4.8\,[eV]$$

The estimated redox potentials and the HOMO, LUMO energy levels are summarized in Table 1. It follows that both compounds exhibit energy levels suitable for use in OPVs. The higher Eg of P3.6C-DTBT-5F (TOL) and of P3.6C-DTBT-Ph (TOL) is caused by its lower molecular weight.

Compound/Solvent	E_{ons}^{red} (V)	E_{ons}^{ox} (V)	Eg (eV)	Homo (eV)	Lumo (eV)
P3.6C-DTBT-Ph (TCE)	-0.94	+0.95	1.89	-5.2	-3.3
P3.6C-DTBT-Ph (TOL)	-1.04	+1.16	2.20	-5.4	-3.2
P3.6C-DTBT-5F (CB)	-1.08	+1.10	2.18	-5.4	-3.2
P3.6C-DTBT-5F (TOL)	-1.16	+1.17	2.33	-5.4	-3.1

Table 1: HOMO/LUMO levels obtained from cyclic voltammetry

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