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A Low-Energy-Gap Organic Dye for High-Performance Small-Molecule Organic Solar Cells

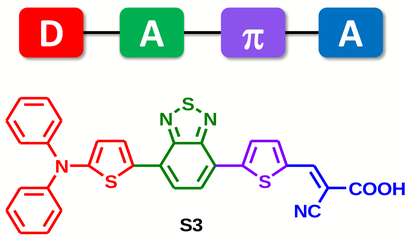
國立台灣大學化學系 博士班三年級 林立彥

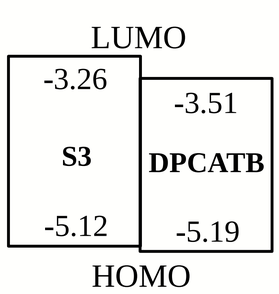
指導教授：汪根欉 博士

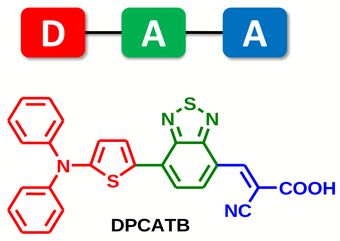
Introduction

Organic solar cells (OSCs) are emerging as a clean and competitive renewable energy resource due to their unique features including low-cost manufacturing, light weight, and mechanical flexibility. Recently, I synthesized and characterized a donor–acceptor–acceptor (D–A–A)-type donor molecule, **DTDCTB**. Vacuum-deposited planar mixed heterojunction (PMHJ) devices employing **DTDCTB** as the electron donor and C_{70} as the electron acceptor achieved power conversion efficiencies (PCEs) of up to 5.81%, which is among the highest values ever reported for vacuum-deposited single cells with organic donor molecules.

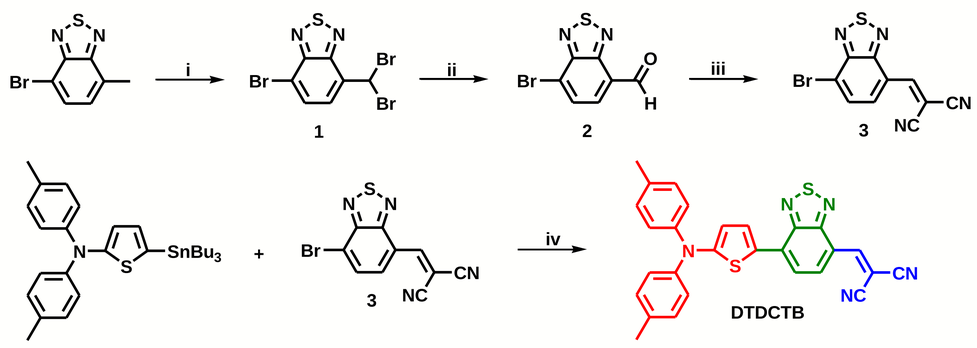
Model Study





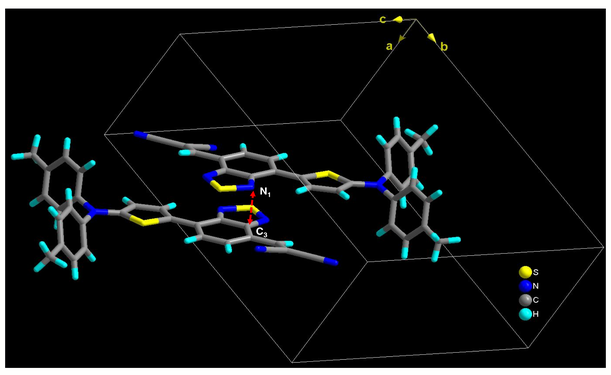


Synthetic Route to DTDCTB



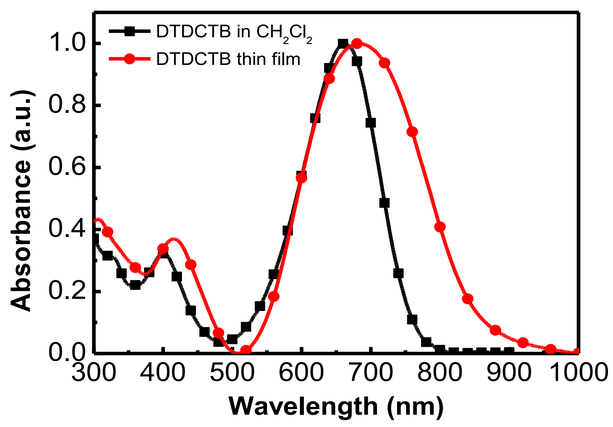
(i) NBS, azobis(isobutyronitrile), chlorobenzene, 80 °C, 83%. (ii) $AgNO_3$, H_2O/MeCN, reflux, 92%. (iii) Malononitrile, Al_2O_3, toluene, 70 °C, 67%. (iv) $PdCl_2(PPh_3)_2$, toluene, 110 °C, 55%.

Crystal Packing



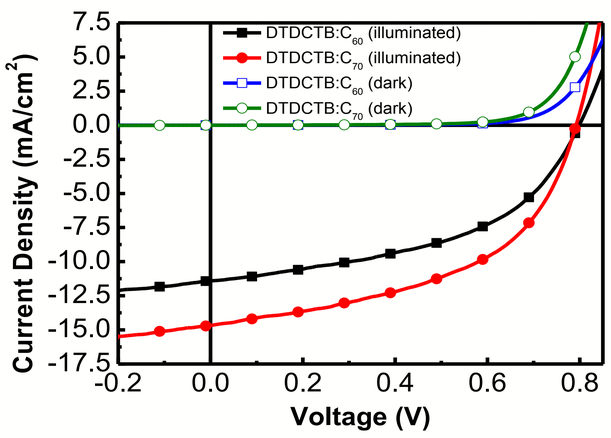
• **antiparallel arrangement**

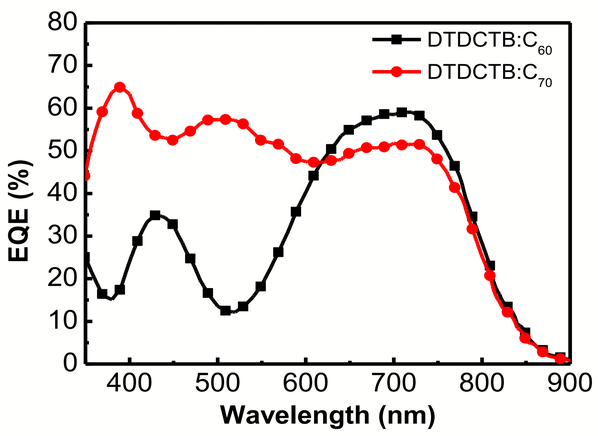
Absorption Spectra



compd	λ_{abs} soln (nm) (ε, M^{-1} cm^{-1})	λ_{abs} film (nm)	k_{max}	ΔE^{opt} film (eV)	E_{ox}^1 (V)	E_{red}^1 (V)	HOMO (eV)	LUMO (eV)
DTDCTB	663 (41660)	684	0.95	1.86	0.35	-1.09	-5.30	-3.44

Photovoltaic Performance





Device Structure : ITO/MoO_3 (5 or 30 nm)/**DTDCTB** (7 nm)/1:1 (v/v) **DTDCTB**:C_{60} or **DTDCTB**:C_{70} (40 nm)/C_{60} (20 nm) or C_{70} (7 nm)/ BCP (10 nm)/Ag (150 nm).

device type	J_{sc} (mA cm^{-2})	Integrated EQE (mA cm^{-2})	V_{oc} (V)	FF	PCE (%)
DTDCTB : C_{60}	11.40	10.97	0.80	0.48	4.41
DTDCTB : C_{70}	14.68	14.26	0.79	0.50	5.81

Conclusion

A D–A–A-type donor material, **DTDCTB**, in which an electron-donating ditolylaminothienyl moiety and an electron-withdrawing dicyanovinylene moiety are bridged by another electron-accepting 2,1,3-benzothiadiazole block, has been synthesized and applied in the fabrication of vacuum-deposited SMOSCs. The innovative structural design strategy enables **DTDCTB** to exhibit distinguished light-harvesting abilities with spectral responses close to the near-IR region. Vacuum-deposited SMOSCs employing **DTDCTB** as the electron donor and C_{70} as the electron acceptor demonstrated exceptional PCEs as high as 5.81% in initial trials. The high efficiency is primarily attributed to the broad and intensive absorption (giving high J_{sc}) and a reasonably low-lying HOMO level (giving high V_{oc}) of the **DTDCTB** thin film. Our results indicate the great potential of such D–A–A systems in creating high-performance donor materials for SMOSCs.

Personal Publications

(1) Lin, L.-Y.; Tsai, C.-H.; Wong, K.-T.*; Huang, T.-W.; Hsieh, L.; Liu, S.-H.; Lin, H.-W.; Wu, C.-C.*; Chou, S.-H.; Chen, S.-H.; Tsai, A.-I *J. Org. Chem.* **2010**, *75*, 4778. (SCI journal, IF: 4.002)

(2) Lin, L.-Y.; Tsai, C.-H.; Wong, K.-T.*; Huang, T.-W.; Wu, C.-C.*; Chou, S.-H.; Lin, F.; Chen, S.-H.; Tsai, A.-I *J. Mater. Chem.* **2011**, *21*, 5950. (SCI journal, IF: 5.099)

(3) Lin, L.-Y.; Lin, X.-Y.; Lin, F.; Wong, K.-T.* *Org. Lett.* **2011**, *13*, 2216. (SCI journal, IF: 5.250)

(4) Lin, H.-W.*; Lin, L.-Y.; Chen, Y.-H.; Chen, C.-W.; Lin, Y.-T.; Chiu, S.-W.; Wong, K.-T.* *Chem. Commun.* **2011**, *47*, 7872. (SCI journal, IF: 5.787)

(5) Lin, L.-Y.; Lu, C.-W.; Huang, W.-C.; Chen, Y.-H.; Lin, H.-W.*; Wong, K.-T.* *Org. Lett.* **2011**, *13*, 4962. (SCI journal, IF: 5.250)

(6) Lin, L.-Y.; Chen, Y.-H.; Huang, Z.-Y.; Lin, H.-W.*; Chou, S.-H.; Lin, F.; Chen, C.-W.; Liu, Y.-H.; Wong, K.-T.* *J. Am. Chem. Soc.* **2011**, *133*, 15822. (SCI journal, IF: 9.019)

(7) Chiu, S.-W.; Lin, L.-Y.; Lin, H.-W.*; Chen, Y.-H.; Huang, Z.-Y.; Lin, Y.-T.; Lin, F.; Liu, Y.-H.; Wong, K.-T.* *Chem. Commun.* submitted.

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