Synthesis and Characterization of Low Bandgap Polymers Containing 2,7-Dibenzosilole for High Open-Circuit Voltage in Organic Solar Cells

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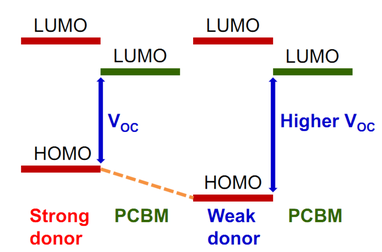
Nanomaterials for Environmentally Friendly Energy Conversion

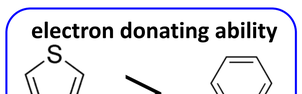
Introduction

❖ Energy level tuning of D–A type polymers

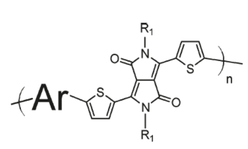


- By introducing weak electron-rich units in conjugated molecules

electron donating ability



→ *deeper HOMO energy levels*



Ar	HOMO (eV)
	–5.17
	–5.35

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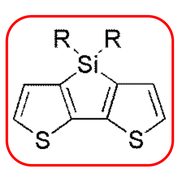
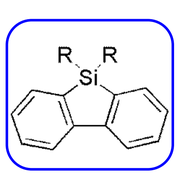
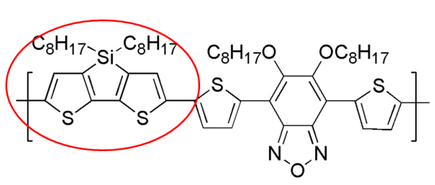
❖ Introduction of dibenzosilole (DBS) instead of dithienosilole (DTS)



- ✓ rigid coplanar structure → *intermolecular π–π interaction*
- ✓ Si bridging atom → *high hole mobility*
- ✓ strong electron donating ability → *high HOMO energy level*

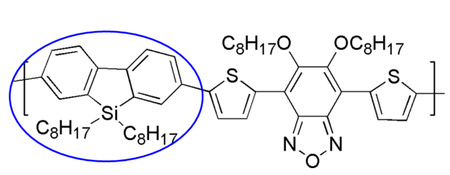


- ✓ coplanar and Si bridging atom → *similar structure of DTS*
- ✓ weak electron donating ability → *low HOMO energy level*



PDTSDTBO

V_{OC} ↑



PDBSDTBO

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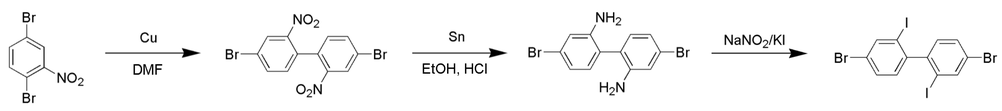
Objectives

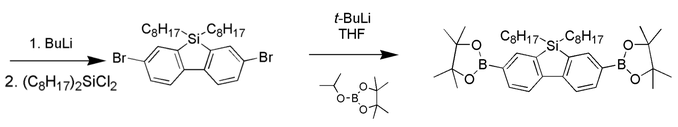
- To synthesize alternating low bandgap copolymer with dibenzosilole and benzooxadiazole for high V_{OC} polymer solar cells
- To compare the photophysical and photovoltaic properties of DBS–based polymers with those of DTS–based ones

Results

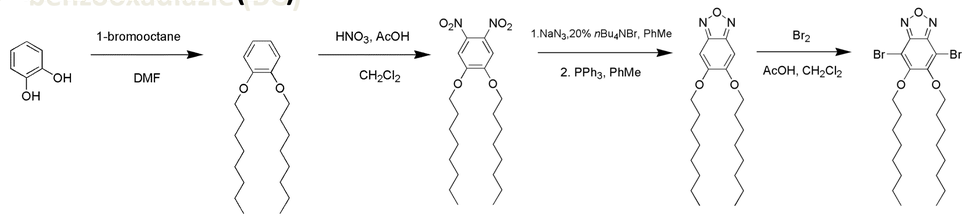
❖ Synthesis of monomers

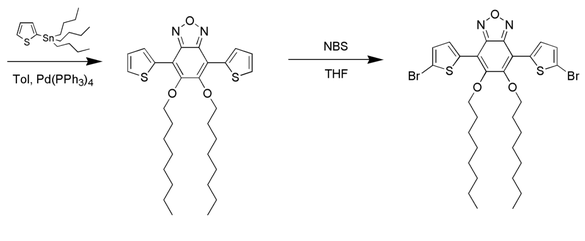
✓ dibenzosilole (DBS)



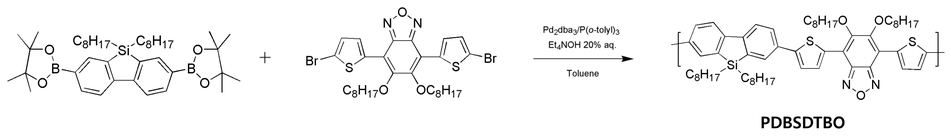


✓ benzooxadiazle (BO)

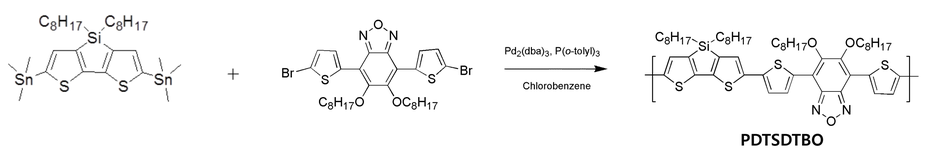




❖ Synthesis of polymers



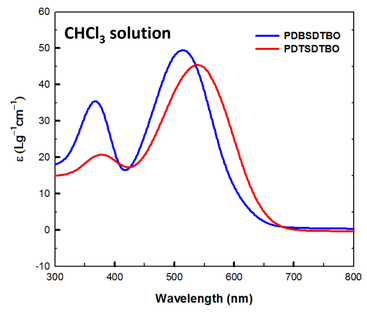
PDBSDTBO

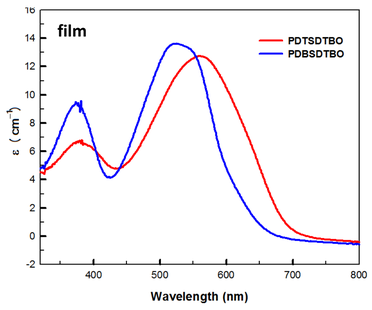


PDTSDTBO

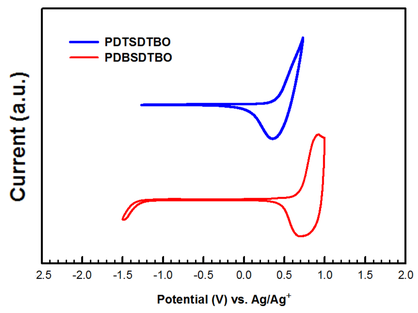
❖ Optical and electrochemical properties of the polymer

✓ UV–vis absorption spectra





✓ Cyclic voltammogram



Polymer	Absorption		E_g^{opt}	HOMO	LUMO[a]
	$\lambda_{max}(CHCl_3)$ (nm)	λ_{max}(film) (nm)	(eV)	(eV)	(eV)
PDTSDTBO	680	740	1.68	-5.2	-3.52
PDBSDTBO	635	660	1.88	-5.5	-3.62

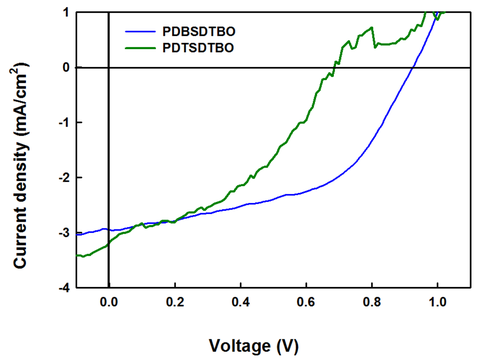
[a]Calculated from $E_{LUMO} = E_{HOMO} + E_g^{opt}$

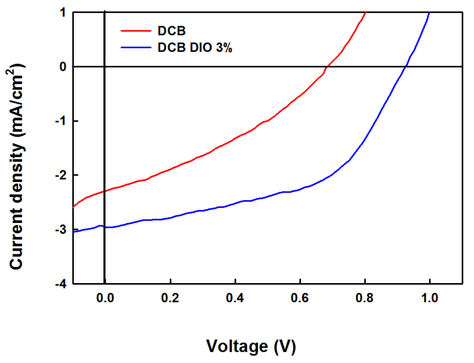
- *Weak electron-donating power of pheylene → Deep HOMO energy level and large bandgap of PDBSDTBO*

❖ Photovoltaic properties of the polymers

✓ solvent: DCB + 2vol%DIO

✓ PDBSDTBO



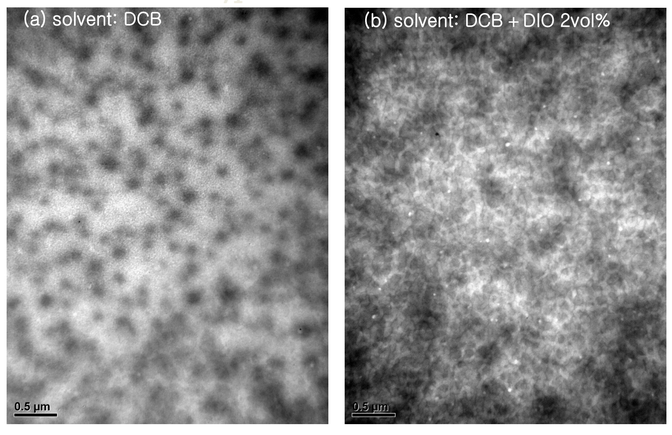


Polymer	Polymer:$PC_{71}BM$ (w/w)	Solvent	V_{OC} (V)	J_{SC} (mA/cm^2)	FF	PCE (%)
PDBSDTBO	1:2	DCB	0.68	2.29	0.34	0.53
PDBSDTBO	1:2	DCB + 2vol% DIO	0.93	2.95	0.51	1.40
PDTSDTBO	1:2	DCB + 2vol% DIO	0.70	3.18	0.40	0.88

- *PDBSDTBO with deeper HOMO energy level show enhanced V_{OC} and PCE*

❖ Morphology of active layers

✓ PDBSDTBO:$PC_{71}BM$ = 1:2



- **(a) solvent: DCB**

  $PC_{71}BM$ aggregation cause charge recombination → low J_{SC}, FF

- **(b) solvent: DCB + DIO 2vol%**

  DIO reduced to $PC_{71}BM$ aggregation → improved morphology

Conclusions

- BO–based low band gap copolymers, PDBSDTBO and PDTSDTBO were successfully synthesized by Suzuki and Stille coupling, respectively
- PDBSDTBO with deeper HOMO energy level showed enhanced V_{OC} (0.93 ev) and PCE (1.40%) than those of PDTSDTBO (V_{OC}: 0.70eV, PCE: 0.88%)
- Further optimization is required by changing solvent to get preferable morphology