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Published in:
Organic Photovoltaics 7

Link to article, DOI:
10.1117/12.679012

Publication date:
2008

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Bundgaard, E., & Krebs, F. C. (2008). Low band gap polymers for organic solar cells. In Z. H. Kafafi, & P. A. Lane (Eds.), *Organic Photovoltaics 7* (Vol. 6334). [63340T] Bellingham: SPIE - International Society for Optical Engineering. Proceedings of SPIE, the International Society for Optical Engineering, Vol.. 6334
https://doi.org/10.1117/12.679012

Low band gap polymers for organic solar cells

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Abstract

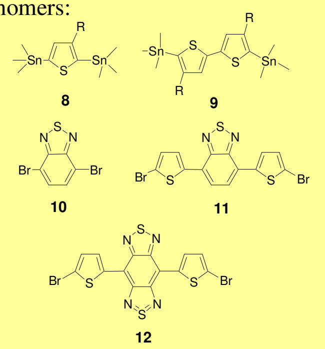
The synthesis of copolymers based on thiophene, benzothiadiazole and benzo-bis(thiadiazole) is presented. The band gaps were estimated from UV-vis and the electron structure of the polymers were determined by Ultraviolet photoelectron spectroscopy (UPS). Results for some photovoltaic devices are given.

Introduction

The use of low band gap polymers for organic photovoltaic are believed to increase the efficiency of the device by a better overlap with the solar spectrum. The synthesis of low band gap polymers are however a challenge and only a few examples have been reported. The most important ones are polythiophene, polyisothianaphthene and copolymers of benzothiadiazole, thiophene and pyrrole with band gaps of 2.0, 1.2 and 1.6 eV, respectively. Here we present the synthesis and characterization of copolymers based on thiophene, benzothiadiazole and benzobisthiadiazole.

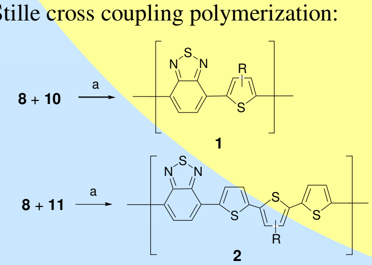
Synthesis

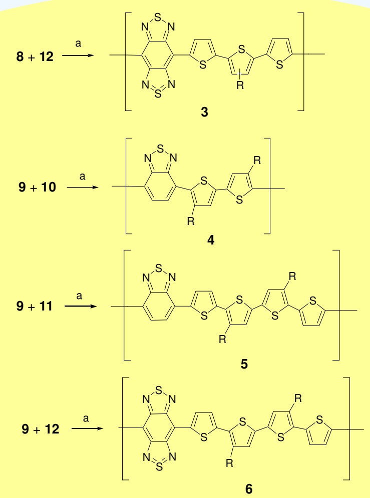
Monomers:



8, 9, 10, 11, 12

Stille cross coupling polymerization:



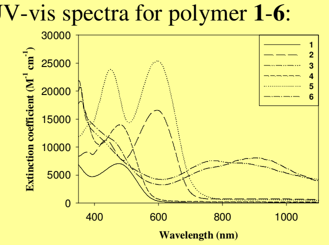


Results

SEC data for polymer **1-6**:

Polymer	M_w	M_{peak}	M_w/M_n
1	5800	4800	1.4
2	2300	2100	1.3
3	7100	8600	1.9
4	9400	9500	1.8
5	14000	12000	1.9
6	12000	11000	2.1

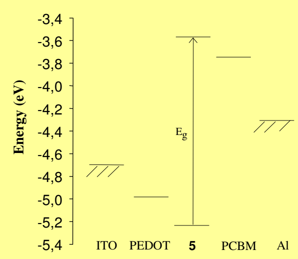
UV-vis spectra for polymer **1-6**:



UPS data for polymer **1-6** (E_g estimated from UV-vis):

Polymer	E_F^{VB} (eV)	E_F^{VAC} (eV)	IP (eV)	Δ (eV)	E_G (eV)
1	1.44	3.96	5.40	-0.64	2.10
2	0.80	4.04	5.84	-0.56	1.82
3	0.52	3.92	4.44	-0.68	0.65
4	1.11	3.81	4.92	-0.79	2.10
5	0.63	4.04	4.67	-0.56	1.65
6	0.48	3.86	4.34	-0.74	0.67

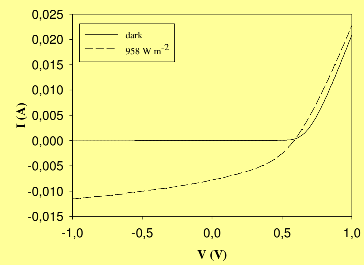
Energy levels in a photovoltaic device with **5** and PCBM:



Photovoltaic devices were prepared with polymer **5** and with a blend of polymer **5** and PCBM. The photovoltaic performance for these devices is summarized in the table below.

Device	V_{OC} (V)	I_{SC} (mA cm^{-2})	FF (%)	η (%)
5, 3 cm^{-2}	0.69	-0.012	25	0.001
5/PCBM (1:2), 3 cm^{-2}	0.58	-2.70	38	0.6
5/PCBM (1:2), 10 cm^{-2}	0.56	-1.29	28	0.2

IV-curve for the polymer **5** and PCBM:



The photovoltaic studies showed:

- I_{SC} increased when PCBM was added.
- Highest η for **5**/PCBM 1:2 ratio.
- I_{SC} and η decreases with increase in area (3 and 10 cm^2 devices).
- Lifetime of less than 2 hours for non encapsulated devices.
- IPCE of 22% at 560 nm for ITO-PDOT-**5**/PCBM (1:2)-Al.

Conclusion

Low band gap copolymers based on thiophene, benzothiadiazole and benzo-bis-thiadiazole were synthesized by Stille cross coupling polymerization and the band gaps were estimated to 2 – 1.7 eV for polymers based on benzothiadiazole and 0.7 eV for polymers based on benzo-bis(thiadiazole).

Polymer **5** was applied in large area photovoltaic devices (3 and 10cm²) with the configuration ITO-PEDOT-**5**/PCBM (1:2)-Al which gave a efficiency up to 0.6%. Further work is in progress to apply all polymers in OPV and to improve the efficiency of the devices with polymer **5**.

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