

ISOINDIGO AS A BUILDING BLOCK FOR SEMICONDUCTING CONJUGATED POLYMERS FOR HIGH PERFORMANCE ORGANIC PHOTOVOLTAICS

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1) Context / Study motivation

One of the most important issues for enhancing the power conversion efficiency (PCE) of polymer solar cells (PSCs) is the development of conjugated polymers which exhibit broad light absorption with strong absorptivity, high charge carrier mobility, suitable energy level matching with the electron acceptor (fullerene derivatives), and appropriate molecular orientation to form an optimum pathway of charge carriers to the corresponding electrodes. In past few years, remarkable progress in the PCE surpassing 8% have been achieved with the configuration of bulk-heterojunction network structure consisting of high performance conjugated polymer as an electron donor and fullerene derivative as an acceptor.

Isoindigo is a dye molecule with two lactam rings pertaining strong electron-withdrawing characteristic and planar π -conjugated structure. Particularly, the planar molecular structure is expected to afford high charge carrier mobility. Moreover, isoindigo-based organic compounds show broad optical absorption, high extinction coefficient, and deep HOMO energy level. Therefore, isoindigo is a promising building block for constructing low bandgap conjugated polymers to achieve high performance PSCs.

2) Description of approach and techniques

We synthesized random conjugated copolymers consisting of DPP and isoindigo as co-electron donor units in donor-acceptor type conjugated copolymer for panchromatic absorption (Scheme 1).

We also synthesized highly π -extended conjugated low bandgap polymer composed of isoindigo (iI) and thienylvinylene (TVT) and compared the photovoltaic properties of PiITVT with those of PiI2T which is an isoindigo-based polymer without vinyl linkage, in order to examine the effect of vinylene linkage on the photovoltaic properties of isoindigo-based

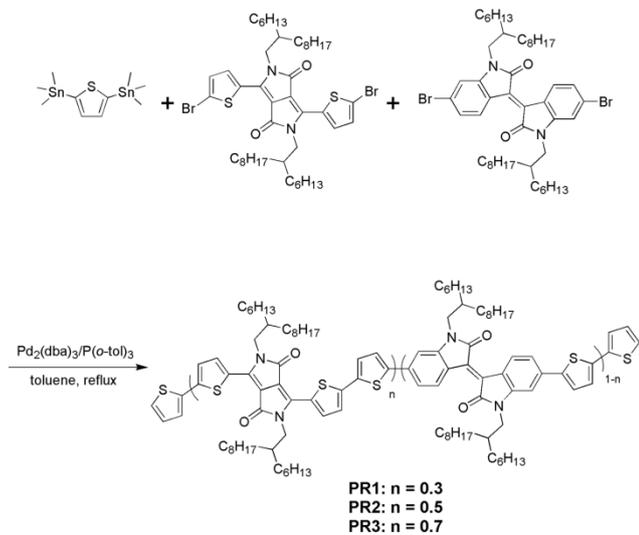
polymers (Scheme 2).

3) Results / Conclusions / Perspectives

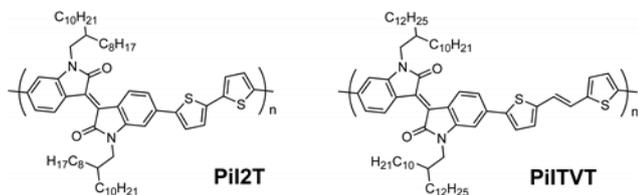
The copolymer containing equal amount of DPP and isoindigo in the copolymer absorbs wide range of solar spectrum from 600 to 900 nm with low HOMO level, which is beneficial for achieving high performance PSCs (Figure 1). Furthermore, the random copolymers have semi-crystalline nature along with preferential face-on orientation on the substrate, which facilitates effective charge transport in vertical direction to the electrode. The morphology analysis reveals that an addition of DIO effectively reduces the domain size, which also contributes to efficient charge transport for high short circuit current (J_{SC}) of PSCs. Under the optimized condition, the copolymer-based PSC exhibits a promising PCE of 6.04% with a V_{OC} of 0.77 V and a J_{SC} of 13.52 mA/cm² and a FF of 0.58, which are superior to the values of the two homopolymers (Figure 2). Therefore, the synthesis of random conjugated copolymer provides a potential approach to achieve high performance organic solar cells with panchromatic light absorption.

When the solar cell device fabricated from PiITVT:PC₆₁BM blend was optimized by varying the mixing ratio of mixed solvent, the device exhibited a PCE of 7.09%, which is much higher than the best PCE of PiI2T:PC₇₁BM blend (Figure 3). The J_{SC} of the optimized device fabricated from PiITVT is higher than that of optimized PiI2T-based device (13.2 mA cm⁻² vs. 10.7 mA cm⁻²) while the V_{OC} and fill factor of both devices are almost the same. External quantum efficiency spectra also identify that PiITVT has higher J_{SC} than PiI2T. This is probably because PiITVT has more favorable molecular and packing structure to transport free charge carriers (Figure 4).

In short, this work clearly shows that isoindigo unit is a promising building block for constructing conjugated polymer to achieve high performance PSCs.



Scheme 1. Synthetic scheme of conjugated random copolymers.



Scheme 2. Chemical Structure of PiI2T and PiITVT.

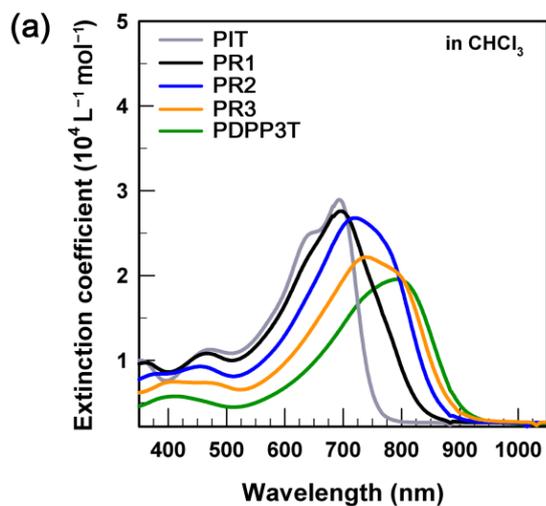


Figure 1. UV-Vis absorption spectra of PIT, PDPPP3T and random copolymers in solution.

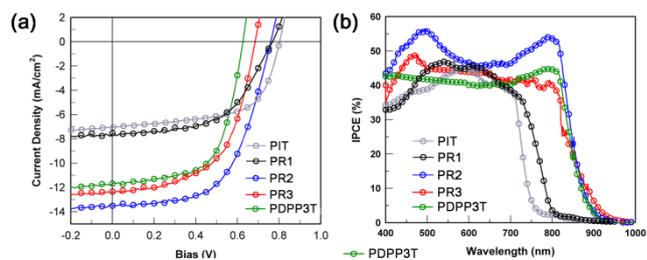


Figure 2. (a) J - V curve and (b) ICPE spectra of the PCEs based on OIT, PDPPP3T and random copolymers.

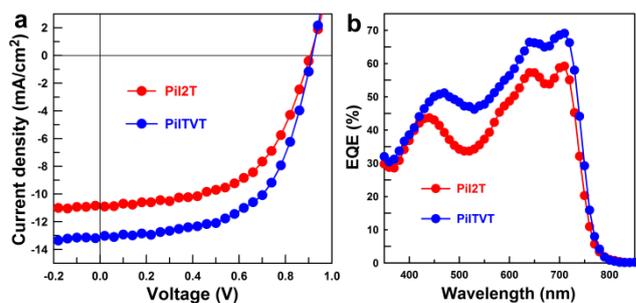


Figure 3. (a) Current density-voltage curves and (b) external quantum efficient spectra of PiI2T:PC71BM and PiITVT:PC61BM bulk heterojunction solar cells under optimized conditions.

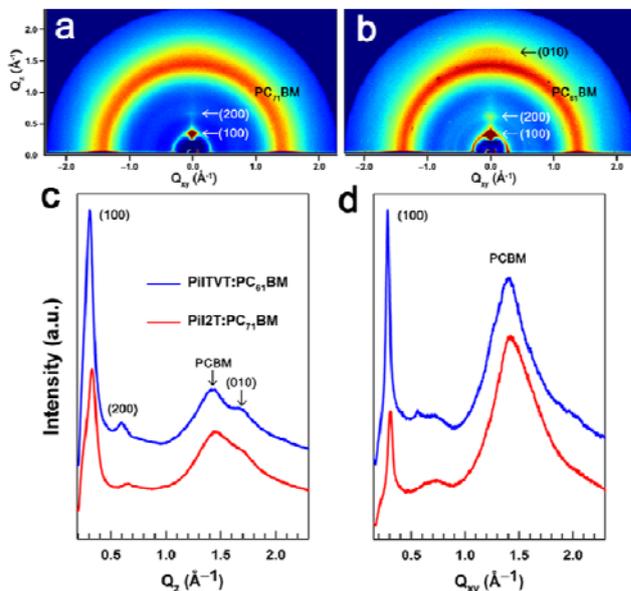


Figure 4. GIWAXS patterns of blend thin films of (a) PiI2T:PC61BM fabricated from CF:DIO (96:4 v/v) and (b) PiITVT:PC61BM fabricated from CF:DCB (9:1 v/v); (c) out-of-plane and (d) in-plane cuts of the corresponding GIWAXS patterns.

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- Marc MEURIS, IMEC, Belgium - "Progress and challenges of CZTSe solar cells for thin film PV applications"
- Thomas KIRCHARTZ, Forschungszentrum Jülich, Germany - "Device Physics of Fullerene Solar Cells"

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THURSDAY, 22ND MAY

8:00am

Welcome Coffee

SESSION 5

PART 1: DYE-SENSITIZED SOLAR CELLS AND ORGANIC PHOTOVOLTAICS

8:30am

Keynote Speaker - **Thomas Kirchartz**, Forschungszentrum Jülich, Germany - **"Device Physics of Polymer: Fullerene Solar Cells"**

9:10am

"Isoindigo as a Building Block for Semiconducting Conjugated Polymers for High Performance Organic Photovoltaics" - **Won Ho Jo**, Eui Hyuk Jung, Jae Woong Jung, Department of Materials Science and Engineering, Seoul National University (Seoul, Korea)

9:30am

"Organic Photovoltaic Tandem Cells : Elaboration, Characterization and Stability" - M. Legros, B. Lechene, R. de Bettignies, CEA, LITEN, Laboratoire des Modules Photovoltaïques Organiques (France), G. Perrier, Laboratoire Optimisation de la Conception et Ingénierie de l'Environnement- CNRS FRE 3220 - Polytech Annecy (Annecy, France), D. Duché, J.-J. Simon, Aix-Marseille University, IM2NP (Marseille, France), N. Lemaitre, S. Berson, CEA, LITEN, Laboratoire des Modules Photovoltaïques Organiques (France)

9:50am

"Analysis of Dynamic Electrical Response of Fresh and Degraded Organic Solar Cells" - S. Altazin, Fluxim AG (Switzerland), S. Züfle, Institute of Computational Physics, Zurich University of Applied Sciences (Switzerland), M. Neukom, Fluxim AG (Switzerland), T. Sauermaann, H. J. Egelhaaf, Belectric OPV GmbH (Switzerland), E. Knapp, Institute of Computational Physics, Zurich University of Applied Sciences (Switzerland), and B. Ruhstaller, Fluxim AG (Switzerland)

10:10am

Break

SESSION 5

FLASH TALK 5 - PART 1 - DYE-SENSITIZED SOLAR CELLS AND ORGANIC PHOTOVOLTAICS

10:40am

Flash Talks, 10:40am - 10:55am. *Have a look on the Flash Talks.*

SESSION 6

SILICON THIN FILM

10:55am

"Iron and Nitrogen Impurities in Laser Crystallised Silicon on Glass Solar Cells" - **J. Dore**, The University of New South Wales- Suntech R&D Australia (Australia), S. Varlamov and M.A. Green, The University of New South Wales (Australia)

11:15am

"Investigation of (I)A-SiO:H Absorber Layers for Use In Triple-Junction