2015 International Chemical Congress of Pacific Basin Societies

DECEMBER 15–20, 2015 • HONOLULU, HAWAII

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455. Adsorption and aggregation properties of homogeneous polyoxypropylene-polyoxyethylene type nonionic surfactants without molecular weight distribution. **S. Yada***, T. Yoshimura

456. Intra- and intermolecular interactions and self-assembly of an amphiphilic alternating copolymer in aqueous solution: complexation with cyclodextrin. **R. Takahashi**, T. Sato, K. Terao, A. Hashidzume

457. Adsorption and aggregation properties of hydrocarbon-fluorocarbon hybrid-type gemini surfactants with carboxylates or quaternary ammonium salts. **T. Yoshimura***, A. Morishima, A. Okuda

458. Supramolecular organogel from amphiphilic cyclic peptide self-assembly in organic solvent. **S. Kanazawa**, I. Akiba*, R. Nakanishi

Hawaii Convention Center
Halls I, II, III

Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281)

Organized by: M. Cunningham, M. Sawamoto, P. Chamapgne, J. Rawlins
Presiding: M. Cunningham

Poster Session
19:00 – 21:00

459. Sustainable monomers and thermoplastic polymers derived from plant oils via amidation. **L. Yuan**, Z. Wang, N. Trenor, C. Tang*

460. Evaluation of dyeing property using regenerated wool fiber. **R. Yasukawa***, S. Asano, K. Sawada

461. Hydrogels based on *Agave tequilana* xylans for wound healing. A. Gonzalez, A. Escalante, E. Delgado, J. González, P. Gatenholm, **G. Toriz***

462. Hemicelluloses-*click*-chitosan polymer stabilized palladium (0) as an active catalyst for Suzuki reactions. C. Wu, **M. Song**, **X. Peng***, L. Zhong, R. Sun

463. Preparation and characterization of polyurethanes derived from biomass based furan-diols. **S. Shin***, H. Ngo

464. Aliphatic polycarbonates based on carbon dioxide, furfuryl glycidyl ether, and glycidyl methyl ether: Reversible functionalization and crosslinking. **M. Scharfenberg**, H. Frey

465. Novel surface wrinkling system with natural resources: Morphology control. **N. Okuda**, S. Ifuku, M. Morimoto, H. Saimoto, H. Izawa*

466. Biosynthesis of Poly(3-hydroxyalkanoate) from amino acids in medium with nitrogen, phosphate, and magnesium, or some combination of these nutrients. **T. NAKAOKI***, M. Sakamoto

467. Novel soft materials derived from green-tide-forming chlorophyta. **K. Kanno**, S. Takahashi, S. Kato, Y. Umeno

468. Preparation of high-molecular-weight aliphatic polycarbonates by condensation polymerization of diol and dimethyl carbonate and Its various applications. **J. Jeon***, B. Lee*

469. Differences in chemical composition and anatomical structure between juvenile wood and mature wood of cultivated *Larix decidua* Mill. from fast growing tree plantations. **A. Jankowska**, P. Boruszewski, A. Kurowska, R. Auriga

470. Copolymerization of epoxides with CO_2 catalyzed by multinuclear cobalt complexes. **Y. Hiranoi**, K. Nakano*

471. Chemical composition of *Populus Hybrida 275* and *Larix decidua* Mill. wood from fast-growing trees plantations as a new type of raw material for wood-based panels industry. **P.J. Boruszewski***, A. Jankowska, R. Auriga, M. Maminski, A. Kurowska, R. Toczylowska-Maminska

472. Polymeric sulfur cathodes based on renewable feedstocks. **A. Melker**, C.J. Hawker

473. Novel surface wrinkling system with natural resources: Mechanism. **H. Izawa***, N. Okuda, S. Ifuku, M. Morimoto, H. Saimoto

474. Ring opening synthesis of polyethylene furanoate (PEF) as a renewable resource based substitute for polyethylene terephthalate (PET). **P. Fleckenstein***, J. Rosenboom*, G. Storti, M. Morbidelli

475. Environment-dependent single-chain mechanics of biomacromolecules and its implications to prebiotic chemical evolution. **S. Cui***

476. Aromatic end-group functionalization as a method to improve mechanical properties of poly(lactic acid). **L. Chile**, A. Wong, P. Mehrkhodavandi*, S.G. Hatzikiriakos*

477. Cyclic carbonate as building block for sustainable synthesis of non-isocyanate polyurethane elastomers. **G. Beniah**, B.E. Uno, N. Wilmot, W.H. Heath, K. Scheidt, J. Torkelson

478. Tailored adhesion of cellulose substrates by surface modification with block copolymers. **J.L. Engström**, F. Hatton, F. D'Agosto, M. Lansalot, E. Malmstrom, A. Carlmark

479. Novel preparation of hybrid thiol-acrylate/thiol-epoxy materials synthesized using a single base-catalyzed cure. **E. Dhulst**, J. Torkelson, W.H. Heath, N. Wilmot

480. Chemical modification on biopolymers for improved functionality in biobased materials. **M.E. Borjesson***

481. Activating polymer production with spinach leaves. **S. Shanmugam***, **J. Xu**, **C. Boyer**

482. Preparation of cationic polymerizable imdazolium ionic liquid-acrylamide copolymer and its corrosion inhibition. **Z. Liu***

483. PPC/PPO selectivity dependency on oxidation state of Co/salcy complex. **M. Hatazawa**, K. Nozaki

484. Enhanced microwave synthesis of nanostructured polyaniline materials. **M. Gizdavic-Nikolaidis***, M. Jevremovic, T. Merian, N. Redon, J. Wojkiewicz, D. Stanisavljev, G. Bowmaker, Z. Zujovic

485. Living polymerization of renewable methylene butyrolactone monomers using oxidatively activated group transfer polymerization initiators. **Y. Zhang***, E. Chen*

486. Natural polymers reinforced with cellulose nanocrystal to protect the antimicrobial properties of active packaging and beads. **m. Iacroix***

487. Crystalline and functional CO_2-based polycarbonates. Y. Liu, W. Ren, **X. Lu***

488. Thermal degradation and stability of starch under different processing conditions. **X. Liu**, S. Zhou

Hawaii Convention Center
Halls I, II, III

Sustainable Conversion of Lignin to Value-Added Products and Green Chemicals (#319)

Organized by: X. Zhang, Q. Guo, W. Qin, T. Hu, K. Ramasamy
Presiding: X. Zhang

Poster Session
19:00 – 21:00

489. Synthesize and characterization of 2-pyrone-4,6-dicarboxylic acid derivatives and their charge-transfer complexes. **K. Hiruko***, Y. Kuwana, R. Takahashi, K. Inoue, Y. Otsuka, M. Nakamura, H. Ogata

490. Structure and electronic properties of the charge transfer complexes based on 2-pyrone-4,6-dicarboxylic acid and similar molecules. **R. Takahashi***, Y. Kuwana, K. Hiruko, G.F. Gagabe, Y. Otsuka, M. Nakamura, H. Ogata

491. Structures and physical properties of charge-transfer complexes using a metabolicintermediate of lignin, 2-pyrone-4,6-dicarboxylic acid. **Y. Kuwana***, R. Takahashi, K. Hiruko, Y. Otsuka, M. Nakamura, H. Ogata, G.F. Gagabe

492. Lignin model compound bioconversion by versatile peroxidase from *B.adusta*: Mathematical modeling and process control. N. Busse, M. Kraume, **P. Czermak**

493. Influence of lignin on the enzymatic hydrolysis of pretreated biomass substrates. **S. Nakagame***, J.N. Saddler

494. Ti and Au/Ti doped mesoporous materials for the oxidative degradation of lignin. **V. Dufaud***, A. Nunes, L. Djakovitch, D. Da Silva Perez

495. Elucidation of structural features on lignin sub-fractions obtained from sequential solvent fractionation. **S. Park***, J. Kim, H. Hwang, J. Moon, J. Lee, J. Choi

496. Copper on electrospray ligin nanosphere: A catalytic system for azide-alkyne cycloaddition reaction under solvent free condition. Z. Zhou, J. Ma, **X. Peng***, L. Zhong, R. Sun*

497. Comparative study on topochemistry of hydrothermal delignification from Japanese cedar and Japanese beech. **M. Takada***, E. Minami, H. Kawamoto, S. Saka

Hawaii Convention Center
Halls I, II, III

Polymers for Energy and Optoelectronic Devices (#361)

Organized by: K. Oyaizu, R. Advincula, D. Choi

Poster Session
19:00 – 21:00

498. Liquid crystal photo-alignment characteristics of polyimide with charge transfer complexes. **S. Sato***

499. Transformation process and mechanism between the α-conformation and β-conformation of conjugated polymer Poly(9,9-dioctylfluorene) in precursor solution. **D. LU**

500. Electrochemical and mechanical properties of polycarbonate/silica nanofiber composite electrolytes. **Z. LI**, H. MATSUMOTO, Y. TOMINAGA

501. Diindeno[1,2-*g*:1',2'-*s*]rubicene: All-carbon nonfullerene electron acceptor for efficient bulk-heterojunction polymer solar cells with high open-circuit voltage. **C. Chen***, H. Chen, C. Chen

502. Anisotropic field-effect mobilities of liquid crystalline conjugated polymers on photoaligned insulators. **J. Bae***, S. Han, K. Song

503. Electrochemical characterization of polycarbonate-based electrolytes for all-solid-state Li batteries. **M. Yajima**, Y. TOMINAGA*

504. New water-soluble and crosslinkable binder based on chitosan for Si anode of Li-Ion batteries. **M. Cho**, Y. Lee*, C. Chen

505. Broad absorbing and low band gap random copolymers for field effect transistor and polymer solar cell applications. V. Tamilavan , **M. Hyun***

506. Screening for improved bulk heterojunction morphologies of organic semiconductor materials through large-scale Hildebrand solubility parameter calculations. **S.R. Kimura**, D. Yoshidome, H.S. Kwak, M.D. Halls

507. Benzo[1,2-b:4,5-b']dithiophene-functionalized hydrogen-bonding oligothiophene: Self-assembly and photovoltaic properties. **X. Lin**, S. Yagai, T. Kizaki, K. Nakayama

508. Theoretical study of morphology and performance of organic photovoltaics. **E. Kawashima***, M. Fujii, K. Yamashita

509. Electrochemical hydrogenation of poly(4-vinylacetophenone) and its application to a hydrogen storage material. **Y. Shimazaki**, R. Kato, K. Oyaizu, H. Nishide*

510. Synthesis and properties of folded π-stacking polymers and their utilization to organic photovoltaic cell. **Y. Naito**, C. Matsuno, S. Funyu, S. Okamoto*

511. Optoelectronic properties of polymer composites doped by fullerene derivatives with electron-donating/accepting functionalization. **F. Kim***, H. Song, K. Park, J. Choi, N. Kim

512. Effects of impurity in amorphous conjugated polymer on performance of organic photovoltaics. **J. Kuwabara**, N. Takase, T. Yasuda, T. Kanbara

513. High performance ambipolar field-effect transistor based on diketopyrrolopyrrole and benzodithiophene copolymer with cyanovinylene linkage. **J. Park**, S. Park, S. Park*

514. Synthesis and characterizations of polyamides and polyimides containing indolo[3,2-*b*]carbazole moiety in main-chain or side-chain. **R. Ueno**, T. Yoshii, T. Mimura, Y. Nagase*, M. Kawamoto

515. Flexible organic photovoltaics on polyethylene terephthalate substrate prepared by low-temperature process. **T. Kuwabara***, W. Xiaofan, T. Yamaguchi, T. Taima, K. Takahashi

516. Synthesis and properties of bisphenol B novolac resin as a photo-resist material. **T. Nishimura**, H. Yamasaki*

517. New electrochromic polymers based on Tröger's base. **W. Li**, T. Michinobu

518. Helix-sense-selective polymerization of 3,5-bis(hydroxymethyl)phenylacetylene bearing rigid and branched aryl groups and their chiroptical properties. **Z. Shi**, M. Teraguchi, T. Aoki, T. Kaneko

519. Simplified electrochemical polymerization to fabricate a PEDOT hole injection/transport layer. **T. Matsushima***, S. Katori, K. Hiroki

520. Synthesis and characterization of poly(arylenevinylenes) by ring-opening metathesis polymerization. C. Yu*, S. Wen, **C. Wang**

521. Electrocatalytic hydrogenation of pyridine polymers and their application to a hydrogen storage material. **T. Ooya**, R. Kato, K. Oyaizu, H. Nishide*

522. Nitrogen atom substitution in benzothiadiazole of conjugated polymer for high performance polymer solar cells. **E. Jung**, J. Jung, j. jo, W. Jo

523. Conjugated random copolymers consisting of pyridine- and thiophene-capped diketopyrrolopyrrole as co-electron accepting unit for efficient polymer solar cells. **J. Lee**, W. Jo

524. Photovoltaic behavior of inverted polymer solar cells using indium tin oxide electrodes modified by piperazine derivatives. **T. Kusumi**, K. Fujimori, T. Kuwabara, T. Yamaguchi, T. Taima, K. Takahashi*

525. Synthesis and characterizations of pendant type poly(acryl amide) containing indolo[3,2-*b*]carbazole moiety. **T. Mimura**, M. Kawamoto, Y. Nagase*

526. Spectroscopic ellipsometry and FTIR-ATR study on removal stage of solvent in spin-coated PEDOT:PSS on crystalline-Si. H. Shirai*, **S. Funada**, Q. Liu, R. Ishikawa, K. Ueno

527. Chemical mist deposition of organic and inorganic films on textured c-Si for efficient crystalline-Si/organic heterojunction solar cells. H. Shirai, **T. Ohki**, K. Ichikawa, H. Jaker, R. Ishikawa, K. Ueno

528. Insight into the energy loss in organic solar cells based on benzotrithiophene copolymers. **E. Al-Naamani**, M. Ide, A. Gopal, A. Saeki*, I. Osaka, S. Seki

529. Carbazole-assisted electrodeposition of graphene oxide. **P. Advincula***, J. Mangadlao, R. Advincula*

530. Spectroscopic studies of curing and alignment mechanisms of photoreactive mesogen molecules. K. Song*, **J. Jung**

531. Molecular engineering of benzothienoisoindigo copolymers allowing highly preferential face-on orientations. **M. Ide***

*** Principle Author**

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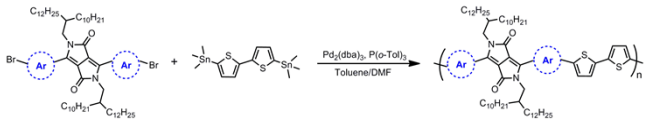
Conjugated Random Copolymers Consisting of Pyridine- and Thiophene-Capped Diketopyrrolopyrrole as Co-Electron Accepting Unit to Enhance Both J_{SC} and V_{OC} of Polymer Solar Cells

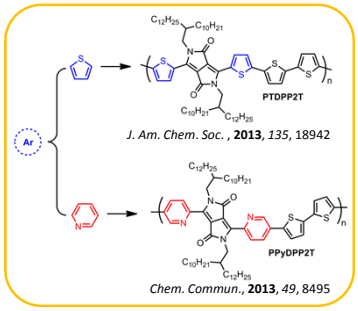
Jong Won Lee, Won Ho Jo*

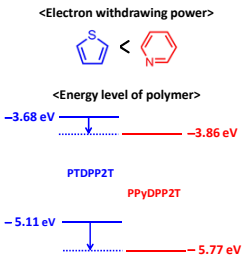
Department of Materials Science and Engineering, Seoul National University, Seoul 151-742, Korea

Introduction

- **Previous research of DPP-based polymer**







Polymer	J_{SC} (mA/cm²)	V_{OC} (V)	FF	PCE (%)
PTDPP2T	**16.00**	0.64	0.69	7.10
PPyDPP2T	7.96	**0.92**	0.65	4.88

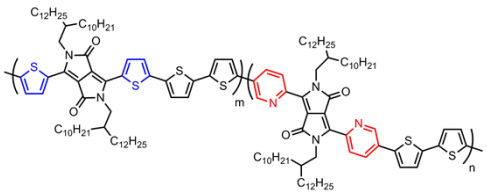
- **PTDPP2T** shows high J_{SC} due to low bandgap, while the **PPyDPP2T** exhibits high V_{OC} due to its low-lying HOMO energy level.

Objectives

- ✓ To synthesize a series of conjugated random copolymers consisting of pyridine- and thiophene-capped diketopyrrolopyroole as co-electron accepting unit
- ✓ To enhance both J_{SC} and V_{OC} of random copolymers by varying the feed ratio of PyDPP to TDPP for copolymerization

Results

❖ Characterization of pristine polymer in this study



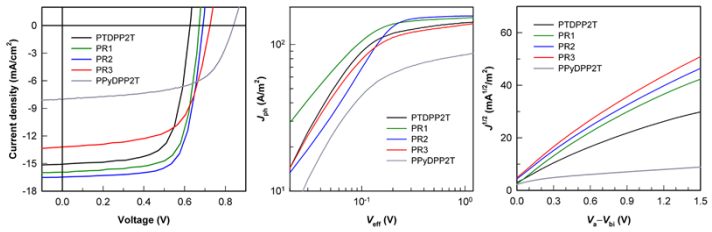
PTDPP2T : m=1, n=0
PR1 : m=4, n=1
PR2 : m=3, n=1
PR3 : m=2, n=1
PPyDPP2T : m=0, n=1

Polymer	M_n (kDa)	PDI	E_g^{opt} (eV)	HOMO (eV)	LUMO (eV)[a]
PTDPP2T	135	1.66	1.32	−5.20	−3.88
PR1	149	1.68	1.35	−5.24	−3.89
PR2	**162**	**1.61**	**1.37**	**−5.30**	**−3.93**
PR3	153	1.66	1.40	−5.32	−3.92
PPyDPP2T	112	1.85	1.60	−5.63	−4.03

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

- The HOMO energy level and bandgap of the polymers become deeper and wider as the PyDPP content in random copolymer is increased.

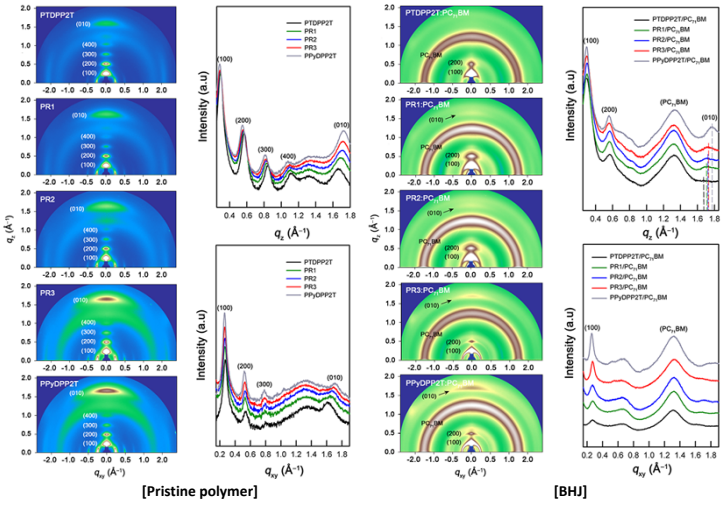
❖ Electrical properties of photovoltaic cells



Polymer	G_{max} (/m³ s)	$\mu_{h,SCLC}$ (cm²/V s)	J_{SC} (mA/cm²)	V_{OC} (V)	FF	PCE (%)
PTDPP2T	7.08×10^{28}	7.76×10^{-3}	15.05	0.63	0.70	6.70
PR1	7.86×10^{28}	1.91×10^{-2}	15.91	0.67	0.71	7.59
PR2	$\mathbf{8.17\times10^{28}}$	$\mathbf{2.72\times10^{-2}}$	**16.44**	**0.69**	**0.71**	**8.11**
PR3	7.60×10^{28}	3.29×10^{-2}	13.51	0.72	0.64	6.29
PPyDPP2T	5.97×10^{28}	4.10×10^{-4}	8.38	0.83	0.59	4.14

- PR2 shows the highest PCE of 8.11% with higher V_{OC} and J_{SC} as compared with PTDPP2T which is due to deep HOMO energy level, higher light absorption and hole mobility.

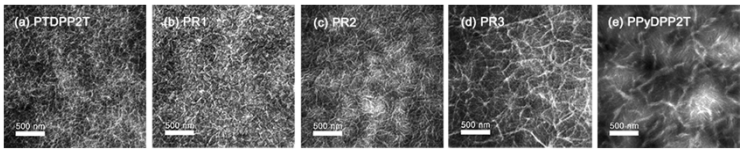
❖ Electrical properties of photovoltaic cells



	Parameters	PTDPP2T	PR1	PR2	PR3	PPyDPP2T
Pristine polymer	q_z (Å^{-1})	1.662	1.688	**1.707**	1.720	1.726
	d-spacing (Å)	3.780	3.722	**3.680**	3.653	3.640
BHJ	q_z (Å^{-1})	1.663	1.702	**1.719**	1.730	1.778
	d-spacing (Å)	3.778	3.691	**3.655**	3.631	3.533

- The intensity of (010) peak in q_z direction increases and the π–π stacking distance decreases, as the pyridine content in polymer backbone is increased.

❖ TEM images



- As the pyridine content in polymer backbone is increased, the fibril width of the polymer becomes larger, which interrupts efficient charge separation from excitons to free charge carriers.

Conclusions

- ✓ The solar cell device based on the random copolymer with the feed ratio of 3:1 (TDPP:PyDPP) shows higher PCE (8.11%) than that of reference homopolymer (6.70%), which is attributed to enhancement of J_{SC} and V_{OC}.

Conjugated random copolymers consisting of pyridine- and thiophene-capped diketopyrrolopyrrole as co-electron accepting unit for efficient polymer solar cells

Jong Won Lee, Won Ho Jo*

Department of Materials Science and Engineering, Seoul National University

One of the most successful approaches to achieve high power conversion efficiency (PCE) of polymer solar cells (PSCs) is to develop new alternating push–pull type copolymers, which consist of electron-rich (D) and electron–poor (A) unit in polymer backbone. Although intensive research efforts have been devoted to developing new D and A moieties, a few D–A alternating copolymers have shown high PCE. Random copolymers composed of one D unit and two different A units can be used as a promising donor material for high performance PSCs, if the absorptions of two electron accepting units are complementary to each other and therefore the resulting copolymer shows broad absorption. Both thiophene-capped (T) and pyridine-capped (Py) diketopyrrolopyrrole (DPP) have been used as electron accepting units for D–A type conjugated polymers for PSCs and OFETs: A low bandgap polymer (pTDPP2T) composed of TDPP and bithiophene (2T) shows high short circuit current due to its low bandgap, while the polymer composed of PyDPP and 2T exhibits high open circuit voltage (V_{OC}) due to its low-lying HOMO energy level. In this work, a new series of conjugated random copolymer was synthesized by copolymerization of 2T (an electron donating unit) with TDPP and PyDPP (co-electron accepting units). The V_{OC} of random copolymer can systematically be controlled by varying the feed ratio of PyDPP to TDPP for polymerization. The V_{OC} was increased with increasing the PyDPP content in the random copolymer, since electron withdrawing power of pyridine is stronger than that of thiophene and thus lower the HOMO energy level: The HOMO energy level becomes deeper as the PyDPP content in the random copolymer is increased. Consequently, the solar cell device based on the random copolymer with the feed ratio of 1:1 shows higher PCE of 7.1% with higher V_{OC} of 0.70 V as compared with those (6.6%, 0.62 V) of the reference homopolymer (pTDPP2T).