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Full paper

Cross-linkable Polymers Containing Triple Bond Backbone and Their Application in Photovoltaic Devices

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Abstract

Two novel polymers containing triple bond in backbone with different conjugated types (acceptor-acceptor, acceptor-donor structures) were synthesized and investigated the crosslinking characteristics under UV irradiation. The crosslink formation was proved via UV-vis and IR spectroscopy, and found that crosslinked polymers have given the solvent resistance properties during the following solvent washing with the similar solvent for active layer. Two triple bond polymers were used as buffer layer materials to modify the interface properties of electron-selective ZnO in the inverted PSCs via spin-coating process. Effects of buffer layer on the surface of ZnO were studied via atomic force microscopy and contact angle measurement. The increased hydrophobic nature of ZnO surface resulted in better contact with active layer, and led to improve the performance of photovoltaic devices with the increased FF.

Keywords: Crosslinkable polymers, triple bond-containing polymers, organic solar cells, inverted solar cells, interlayer.

1. Introduction

Because of many advantages such as lightweight, low cost, flexible substrates, etc. bulk heterojunction (BHJ) organic solar cells (OSCs) have attracted considerable attention recently. During the past decade, the power conversion efficiency (PCE) has been increased significantly and reached over 11% by the use of novel polymer and control of the active layer morphology.^{1,2} In general, the fabrication of multilayer organic electronic devices including OSCs is carried out by one of two methods: high-vacuum vapor deposition or solution processing. The high vacuum vapor deposition can be used for most small molecule-based devices but relatively expensive, time consuming, difficult to make large-area devices and apply for high-molecular weight materials.³ In contrast, solution process have potential in facilitate rapid and low-cost processing, in fabricate in large-size scale, and can be used for all soluble materials. However, during the multilayer integration, the deposition of second layer from solution can lead to partial dissolve the previous layer if the solvent for second layer materials also dissolves the first layer materials.⁴ This is the big challenge for the solution processing method to fabricate multilayer devices by compared to high-vacuum vapor deposition method. To overcome this, a number of efforts have been explored. One of the approaches is developing novel materials that can provide excellent solvent resistance after thermo- or photo-crosslinking or chemical treatments.^{5,6} These cross-linkable materials can be used as electrode buffer layer materials^{7,8} to modify interfacial properties of charge transporting layer of organic electronic devices.

In the past, triple bond containing polymers in the pendant or backbone were found to easily undergo crosslinking on exposure to ultraviolet light and the crosslink reaction could also be sensitized by additives.^{9,10} The formation of only a few fractions of crosslinks is probably sufficient to insolubilize the polymer. So, triple bond containing polymer is one of the potential candidates as the crosslinkable material which can be used for fabricating multilayer devices by solution processing. In this regard, we firstly tried the synthesis of a series of polymers containing triple bond with different conjugated backbone structure, donor-acceptor (D-A), donor-donor (D-D), and acceptor-acceptor (A-A). Two polymers, D-A and A-A, were tested the crosslinkability under UV irradiation. We expected the crosslinked layer was not washed out when the next layer was introduced. Then these polymers were used as buffer layers on top of ZnO to improve the performance of inverted polymer solar cells (PSCs).

2. Experimental section

2.1. Instruments and characterization

Molecular weights were determined with GPC on Viscotek TSA302 Triplet Detector Array system in CHCl_3 using polystyrene standard at room temperature. Absorption spectra were recorded on a Shimadzu UV-3600 UV-visible spectrometer. The samples for UV-vis absorption measurements were prepared by spin-coated the solution of polymer in chloroform on cleaned quartz glass substrates. CV was measured by using IviumStat instrument. CV is conducted with a scan rate of 50 mV s^{-1} at room temperature under the protection of argon with 0.1M tetrabutylammonium tetrafluoroborate in acetonitrile as the electrolyte. A platinum electrode was coated with a thin copolymer film and used as the working electrode. A Pt wire was used as the counter electrode, and a Ag/AgNO_3 (0.1 M) electrode was used as the reference electrode.

2.2. Fabrication and characterization of polymer solar cells

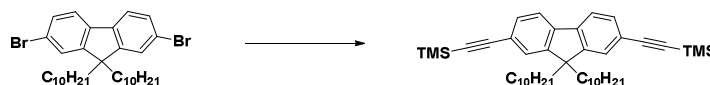
The structure of BHJ device is ITO/ZnO/Interlayer polymer/P3HT:PC₆₁BM (1.0:0.8 w/w)/MoO_x/Al. To fabricate PSCs, first, ITO coated glass slides were cleaned by detergent, followed by ultrasonic washing in D.I. water, acetone and IPA subsequently, and dried in an oven overnight. After UV-ozone treatment for 10 min, ZnO solution was spin-coated onto the ITO substrate at 6000 rpm for 40 s and then annealed at 200 °C for 1 hour. For deposition of the active layer, P3HT:PC₆₁BM (1.0:0.8 w/w) dissolved in o-DCB were spin-cast on top of the ZnO layer in a nitrogen-filled glove box. Finally, metal top electrode, MoO_x and Ag, were sequentially deposited onto BHJ active layer in vacuum ($< 2 \times 10^{-6}$ Torr) by thermal evaporation.

The J - V characteristics of the devices were recorded by solar simulator using Keithley 2400 source measure unit. The characterization of un-encapsulated solar cells was carried out in air under illumination of AM 1.5G, 100 mW cm^{-2} , using a solar simulator (McScience, Inc.) with xenon light source. Illumination intensity was set using an NREL certified silicon diode with an integrated KG5. The external quantum efficiency (EQE) was measured using a reflective microscope objective to focus the light output from a 100 W halogen lamp outfitted with a monochromator and an optical chopper (McScience, Inc.).

2.3. Materials

2,7-Dibromo-9,9-didecylfluorene;¹¹ 4,7-bisethynyl-2,1,3-benzothiadiazole;¹² 2,5-bis(5-bromo-3-hexylthiophene-2-yl)thiazolo[5,4-d]thiazole;¹³ N-heptadecan-9'-yl-2,7-dibromocarbazole¹⁴ were synthesized according to the procedures reported in the literature. Other reagents and solvents were purchased from Sigma Aldrich, Tokyo Chemical Industry Co., LTD and 4Chem Laboratory. All chemicals were used as received. Other monomers were synthesized according to **Scheme 1**.

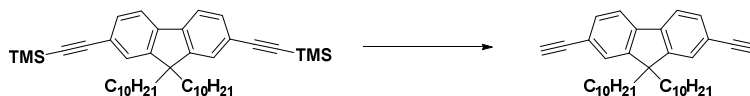
Preparation of 2,7-bis(2-trimethylsilyl)ethynyl-9,9-didecylfluorene



A mixture of 2,7-dibromo-9,9-didecylfluorene (12.090 g, 20 mmol), tetrakis (triphenylphosphine palladium (0)) (0.464 g, 0.4 mmol), copper (I) iodide (0.152 g, 0.8 mmol) and trimethylsilyl acetylene (5.893g, 60.00 mmol) was dissolved in 140 mL triethylamine. The reaction mixture was stirred at 75 °C for overnight under Ar atmosphere. After cooled to room temperature, the solvent of reaction was removed under reduced pressure. The residue was extracted with CH₂Cl₂. The organic layer was washed with cool water and aqueous 1.2 N HCl then dried over anhydrous MgSO₄, and finally evaporated under reduced pressure. The crude was purified by silica gel column chromatography eluting with CH₂Cl₂/hexane (1:4) to obtain 2,7-bis(2-trimethylsilyl)ethynyl-9,9-didecylfluorene (12.66 g, 99%) as the yellow oil.

¹H-NMR (300 MHz, CDCl₃, δ ppm): 7.60 (d, 2H), 7.46 (dd, 2H), 7.42 (s, 2), 1.77-1.71 (m, 4H), 1.12-0.83 (m, 32H), 0.72-0.64 (t, 6H), 0.40 (s, 18H)

Preparation of 2,7-bisethynyl-9,9-didecylfluorene



A mixture of 2,7-bis(2-trimethylsilyl)ethynyl-9,9-didecylfluorene (12.660 g, 19.80 mmol) in 500 mL of 1 mol L⁻¹ KOH methanol solution was stirred at room temperature in the dark for 1 hour. The reaction mixture was poured into cool water (1000 mL) and extracted with CH₂Cl₂ several times. The combined organic layers were dried over anhydrous MgSO₄ and then removed solvent. The residue was further purified by using silica gel column chromatography (hexane as

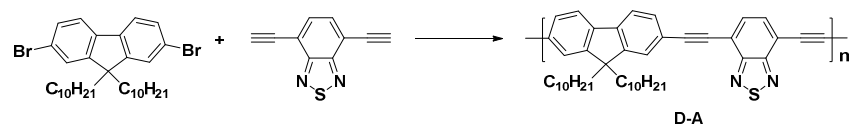
an eluent) to afford 2,7-bis ethynyl-9,9-didecylfluorene as yellow oil (8.56 g, 87%). This compound was stored in the dark under nitrogen at 10°C.

¹H-NMR (300 MHz, CDCl₃, δ ppm): 7.60 (d, 2H), 7.45 (d, 2H), 7.41 (s, 2), 3.06 (s, 2H), 1.77-1.71 (m, 4H), 1.12-0.89 (m, 32H), 0.72-0.64 (t, 6H)

General procedure to synthesize polymers containing triple bond

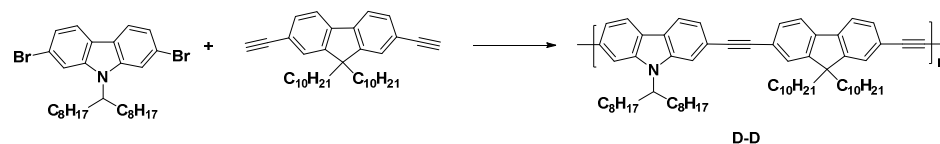
In a sealed tube, diromo-compound (1 eq.), bisethynyl-compound (1 eq.), Pd(PPh₃)₄ (0.1 eq.) and CuI (0.2 eq.) were dissolved in mixed solvent of THF and triethylamine (TEA) (2/1, v/v) under nitrogen atmosphere. The mixture was further frozen, evacuated, and thawed three times to further remove oxygen in the solvent. Then the mixture was stirred at 90 °C in the dark for 48 h. After the resulting solution was cooled down to room temperature, it was then poured into methanol (300 mL). The resulting precipitate was collected by filtration, and the product was further purified by Soxhlet extraction with methanol, acetone and CHCl₃ successively. The CHCl₃ extraction was removed solvent and then precipitated by methanol. Finally, it was collected by filtration and dried in vacuum oven.

Preparation of poly[9,9-bisdecylfluorene-2,7-diyl-ethynylene-alt-4,7-(2,1,3,-benzothiadiazole)] (D-A polymmer)



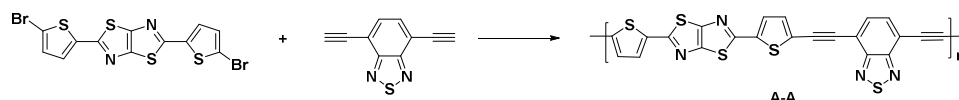
2,7-Diromo-9,9-didecylfluorene (241.1 mg, 0.40 mmol), 4,7-bisethynyl-2,1,3-benzothiadiazole (73.7 mg, 0.40 mmol), Pd(PPh₃)₄ (46 mg, 0.04 mmol) and CuI (15 mg, 0.08 mmol) were dissolved in mixed solvent of THF (3.4 mL) and TEA (1.7 mL) under nitrogen atmosphere. The D-A polymer was obtained as brown solid (125 mg, yield 50%). Mw = 12.2 kg/mol, PDI: 1.487.

Preparation of poly(N-heptadecan-9'-yl-carbazole-2,7-diyl-ethynylene-9,9-bisdecylfluorene) (D-D polymer)



2,7-Bisethynyl-9,9-didecylfluorene (203.4 mg, 0.40 mmol), N-heptadecan-9'-yl-2,7-dibromocarbazole (225.4 mg, 0.40 mmol), Pd(PPh₃)₄ (46 mg, 0.04 mmol) and CuI (15 mg, 0.08 mmol) were dissolved in mixed solvent (THF (5 mL) and Et₃N (1.7 mL)) under nitrogen atmosphere. The D-D crude polymer was obtained as yellow solid, but insoluble in common chlorinated solvent (CHCl₃, CB, o-DCB...) even at hot condition.

Preparation of poly[2,5-bis(5-yl-3-hexylthiophene-2-yl)thiazolo[5,4-d]thiazole-ethynylene-alt-4,7-(2,1,3,-benzothiadiazole)] (A-A polymer)



2,5-Bis(5-bromo-3-hexylthiophene-2-yl)thiazolo[5,4-d]thiazole (253.0 mg, 0.40 mmol), 4,7-bisethynyl-2,1,3-benzothiadiazole (73.7 mg, 0.40 mmol), Pd(PPh₃)₄ (46 mg, 0.04 mmol) and CuI (15 mg, 0.08 mmol) were dissolved in mixed solvent of THF (3.4 mL) and Et₃N (1.7 mL) under nitrogen atmosphere. The A-A polymer was obtained as purple solid (70 mg, yield 27%). Mw = 14.0 kg/mol, PDI: 2.576.

3. Results and discussion

3.1. Material synthesis

The synthetic routes of monomers and corresponding polymers are illustrated in **Scheme 1**. The polymers were obtained by Sonogashira cross-coupling reaction between dibromo- and bisethynyl-compounds in the presence of Pd(PPh₃)₄ and CuI as catalysts and solvent system of triethylamine (TEA)/ THF (1:2, v/v) via thermal heating for 48 hours to obtain D-A, D-D and A-A polymers. However, after reaction, D-D crude product was insoluble in chloroform so we could not purify and investigate further. Two crude polymer products of D-A and A-A were precipitated in MeOH and purified by Soxhlet extraction. The pure polymers D-A and A-A collected from chloroform fraction display high solubility in chlorinated organic solvents such as chlorobenzene (CB), o-dichlorobenzene (o-DCB), chloroform. The yields of polymerizations to synthesize D-A and A-A polymers are 50% and 27%, respectively. The number-average molecular weight (M_n) of D-A and A-A are 12.2 and 14.0 kg mol⁻¹, with polydispersity indexes (PDIs) of 1.487 and 2.576, respectively, as determined by gel permeation chromatography (GPC) using chloroform as an eluent calibrated with polystyrene standards.

From the UV spectra of pristine films (**Figure 1**), the optical properties of two polymers are summarized in **Table 1**, and the band gaps of D-A and A-A polymers were calculated to be 2.25 and 1.90 eV, respectively.

3.2. Crosslinkability of the polymers

Crosslinkability of D-A and A-A polymers were investigated via UV-vis spectroscopy and Infrared (IR) spectroscopy. Crosslink was performed by using UV-irradiation with wavelength of 254 nm. First, the neat polymer films, prepared by spin-coating on quartz substrates, were exposed on UV light with wavelength of 254 for 10 min under inert gas. After that, these treated films were measured by UV-vis spectroscopy before and after rinsed by chloroform. Another polymer film without UV treatment was also rinsed with chloroform and measured UV-vis spectra for comparison. **Figure 1** shows the UV-vis spectra of polymer thin films under different conditions: pristine, rinsed with chloroform, exposed on UV, rinsed with chloroform after exposed on UV. In both case of polymers, the absorption spectrum which observed in pristine films are almost disappeared after rinsed by chloroform. That means, neat thin films can be mostly washed out by the solvent used for the following spin coating. However, the films

exposed by UV light maintained most of UV-vis absorption after rinsed with chloroform. So the generation of cross-linked network seems to be made by exposing UV light. These cross-linked layers will allow subsequent active layer introduction by spin-coating without destroying them.

To prove the cross-linking, IR spectroscopy is performed. The thin films of polymers were fabricated on the surface of KBr plates and measured IR spectra before and after UV exposure to see the change of vibrational stretching of alkyne functional groups in the polymer backbone. As can be seen in **Figure 2**, the vibrational stretching of C≡C group in triple bond at 2191 cm⁻¹ (A-A) and 2192 cm⁻¹ (D-A) were significantly reduced after the UV irradiation, proving the occurrence of cross-linking. The changes of UV spectra shape after UV exposure also support the structural change of polymers.

3.3. Electrochemical properties

To determine the energy levels of synthesized polymers, cyclic voltammetry (CV) is used. The result is shown in **Figure 3** and **Table 1**. For calibration, the redox potential of ferrocene/ferrocenium (Fc/Fc⁺) is measured and it is located at 0.22 V to the Ag/AgNO₃ (0.1 M) electrode. It is assumed that the redox potential of Fc/Fc⁺ has an absolute energy level of -4.8 eV to vacuum.¹⁵ Then the energy levels of the highest occupied molecular orbital (HOMO) is then calculated according to the following equation: $E_{\text{HOMO}} = -(4.58 + E_{\text{ox onset}})$ (eV) and the lowest unoccupied molecular orbital (LUMO) is calculated from E_{HOMO} and optical band gap according to the following equation: $E_{\text{LUMO}} = (E_{\text{HOMO}} + E_{\text{g}}^{\text{opt}})$ (eV). The first oxidation potential of the D-A was appeared at $E_{\text{ox}} = + 1.38$ V (versus Ag/Ag⁺) while in the case of A-A, it was appeared at $E_{\text{ox}} = + 0.75$ V (versus Ag/AgNO₃ (0.1 M)), corresponded the HOMO energy levels of D-A and A-A are -5.96 and -5.33 eV, respectively. Meanwhile, the LUMO energy levels of D-A and A-A were calculated to be -3.71 and -3.43 eV, respectively.

3.4. The effect of buffer layer on the properties of ZnO surface.

To characterize the ZnO surface before and after using buffer layer with UV treatment, AFM images were measured and shown in **Figure 4**. The roughness of ZnO surface are not much affected by the coating of A-A polymer buffer layer, the root mean square (RMS) roughness of neat ZnO, ZnO with A-A buffer layer, and ZnO with A-A buffer layer with UV exposure are 0.927, 1.080, and 0.996 nm, respectively. However, in the case of D-A-based buffer layer, the roughness are significantly increased with the values of 1.551, 1.990 nm, respectively, for the

without and with UV irradiation after D-A polymer introduction on top of ZnO surfaces. The surface of A-A polymer introduced buffer layer showed the fabric network after UV exposure which may be formed from the A-A crosslinked polymers, while in the case of D-A polymer, big grains were formed, led to significantly increased roughness.

The hydrophilicity of the ZnO surface was compared before and after spin-coating buffer layer via the contact angle measurement using water drop, as shown in **Figure 5**. The contact angle was changed from 55.27° to 86.81° (with A-A polymer) and to 75.24° (with D-A polymer) when buffer layer was applied on the top of ZnO. After UV exposure, A-A crosslinked polymer has contact angle value of 82.65° , which is not much different to the before UV irradiation case, while for the case of D-A crosslinked polymer, the contact angle clearly decreased to 66.69° . The maintaining the hydrophobic and smoother surface of A-A polymer was caused by the good surface coverage of crosslinked buffer layer. But reduced hydrophobicity and increased surface roughness of D-A polymer means the surface of ZnO was not fully covered with buffer layer. And this mal-distributed buffer layer of D-A polymer may reduce FF of the devices.

It is well known that the presence of buffer layers in PSCs affects the work function (WF) of electrodes.¹⁶ To investigate this effect, the WFs of the neat ZnO, polymer coated ZnO, and polymer coated ZnO after UV treatment were measured by using ultraviolet photoelectron spectroscopy (UPS), as shown in **Figure 6**. The WF value of neat ZnO was calculated to be 3.69 eV, while the WF values of ZnO coated with D-A and A-A polymers were increased to be 3.75 and 3.70 eV, respectively, and further increased to 3.95 and 3.85 eV, respectively, after 5 min UV exposure. This result means that the WF of the cathode has been down-shifted after coating polymers and UV exposure.

3.5. Photovoltaic characteristics

To study the effect of crosslinked polymer on the photovoltaic performance of inverted OSCs, two kinds of inverted PSCs were fabricated with the configuration of ITO/ZnO/active layer/MoO_x(10nm)/Ag(100nm) and ITO/ZnO/crosslinked polymer/active layer/MoO_x(10nm)/Ag(100nm). The active layer materials were used P3HT as a donor and PC₆₀BM as an acceptor with the weight ratio of 1:0.8 in o-DCB. CB solvent was used to make the solution of crosslinkable polymers. The optimal concentrations of solutions to spin-cast buffer layer were investigated and found to be 2 mg/mL for the case of D-A polymer and 4 mg/mL for

the case of A-A polymer. **Figure 7a** and **7b** show the J-V curves of PSCs under the condition of AM 1.5 at 100 mW cm^{-2} , and the open circuit voltage (V_{OC}), short-circuit current density (J_{SC}), fill factor (FF), and PCE values are summarized in **Table 2**.

The PSC with bare ZnO layer showed an average PCE value of 2.74 % with V_{OC} of 0.61 V, J_{SC} of 8.94 mA cm^{-2} , and FF of 50%. With D-A polymer interlayer, the PCE of the device was improved to 2.91% with V_{OC} of 0.62 V, J_{SC} of 8.90 mA cm^{-2} , and FF of 53%, even without UV exposure. On the other hand, non-UV treated A-A polymer interlayer device case, the PCE was only slightly increased with the value of 2.78%, V_{OC} of 0.61 V, J_{SC} of 8.15 mA cm^{-2} , and FF of 56%. In overall, even without crosslinking, the average PCE were increased in both A-A and D-A polymers in accordance with the improved FF. To investigate the effect of crosslinked polymer buffer on the PSC performance, the A-A and D-A polymer layers were exposed under UV lamp for 5 min after spin-coating. In the case of D-A polymer based device, the average PCE dropped significantly to 2.25% after 5 min UV irradiation of buffer layer, mainly cause by the sharply reducing of FF from 53% to 41%, respectively. On contrast with the trend of D-A polymer, the UV treatment of A-A polymer increased the PCE of the PSC devices. After 5 min UV treatment, the PSC performance of A-A polymer based device showed the PCE value of 3.10% with the increasing of J_{SC} and FF.

In literature, there are many reports about the effect of the work function of two electrodes to the V_{OC} value,¹⁷⁻¹⁹ and the shifting of energy levels of electrodes was used to explain the change in V_{OC} values of PSCs. However, in the case of ZnO with triple bond coating, although the work function of ZnO buffer layer was changed after coating with triple bond polymer (without and with UV treatment), the V_{OC} was not significantly affected. This phenomenon recently was reported and explained by the lower conductivity of the metal oxide (ZnO) layer than those of metal and transparent electrode.²⁰

4. Conclusions

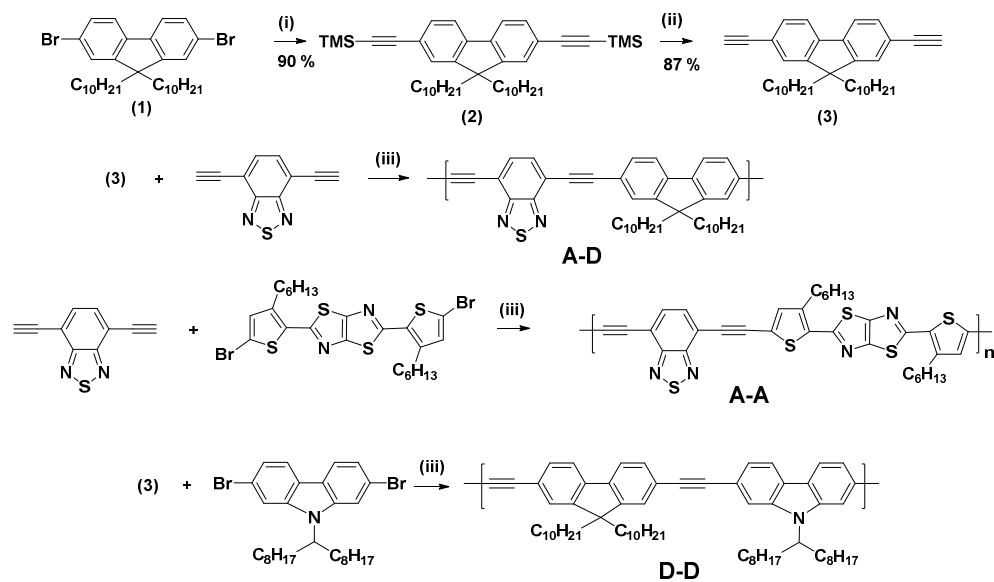
Three novel triple bond containing polymers, named A-A, D-A and D-D, were designed and two of them, A-A and D-A polymers, were investigated their photocrosslikability, as well as their application as buffer layers in OPV. The occurrence of crosslinking was proved by using UV-vis spectroscopy and IR technique. The PSC device with A-A polymer buffer layer exhibited the best average PCE of 3.10% after 5 min UV exposure, caused by the improved FF compare to the device with bare ZnO layer. Our research introduced potential candidates for new photocrosslinkable materials which has solvent resistance and hydrophobic nature, and can be used in solution processed multilayer of organic electronic devices.

Acknowledgments

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Scheme 1. Synthetic routes of monomers and polymers.

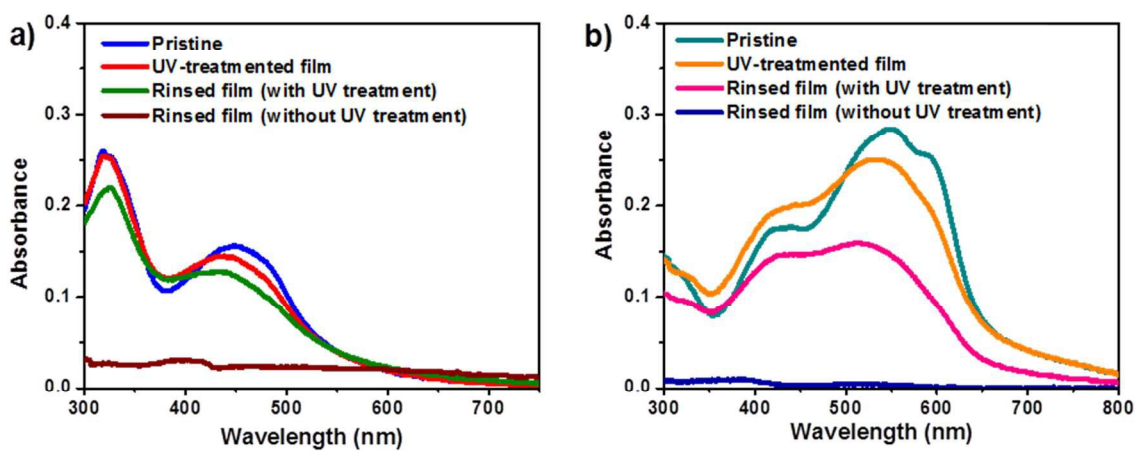


Figure 1. UV-vis absorption spectra of thin films of polymers, a) D-A polymer, b) A-A polymer

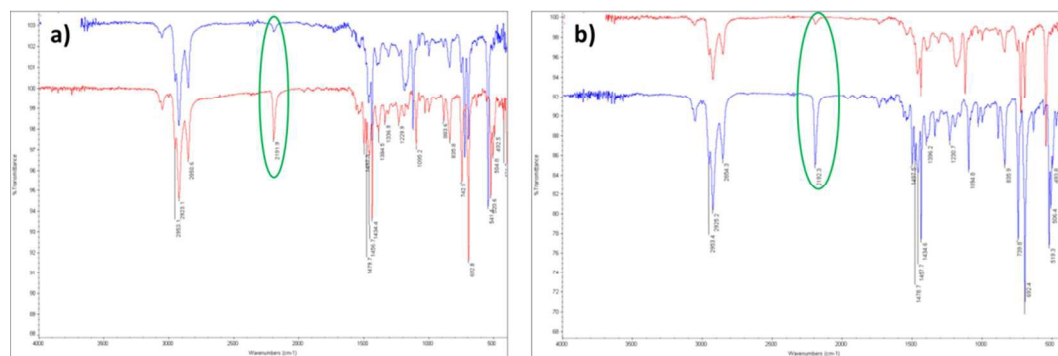


Figure 2. Fourier transform infrared (FT-IR) spectra of a) D-A and b) A-A polymers before (under line) and after (above line) UV treatment.

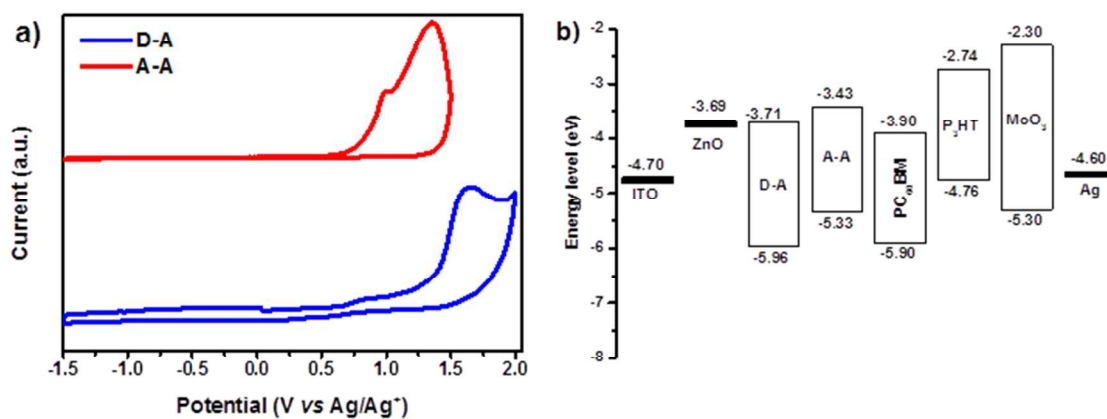


Figure 3. a) Cyclic voltammograms and b) energy levels of the device components.

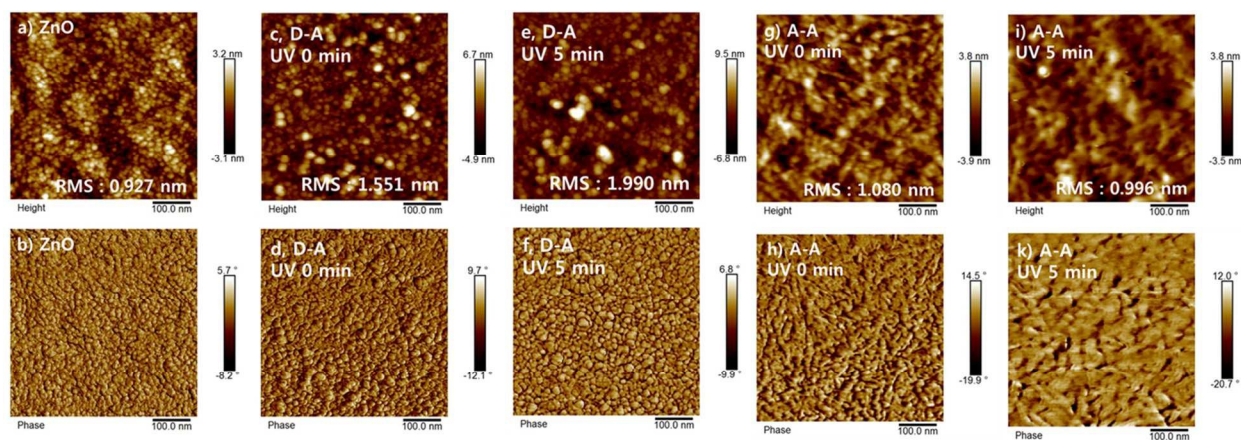


Figure 4. a, c, e, g, i for height images and b, d, f, h, k for phase AFM images of pristine ZnO surface and polymer coated ZnO surfaces without and with UV treatment.

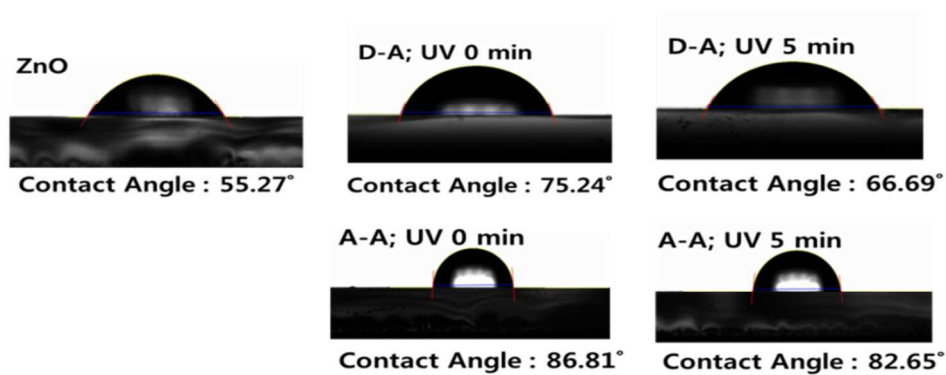


Figure 5. Images of the water contact angle in neat ZnO and treated ZnO.

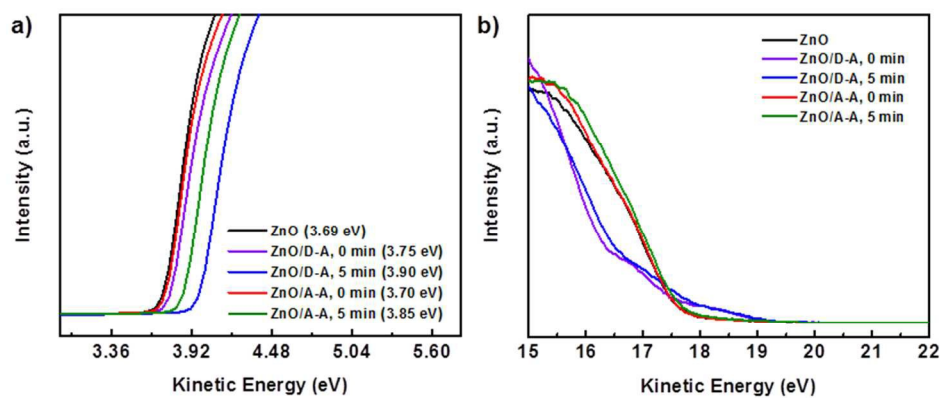


Figure 6. Work functions (a) and fermi-edge region (b) of neat ZnO and polymer coated ZnO without and with UV treatment determined by UPS studies with He ($h\nu=21.2$ eV) source.

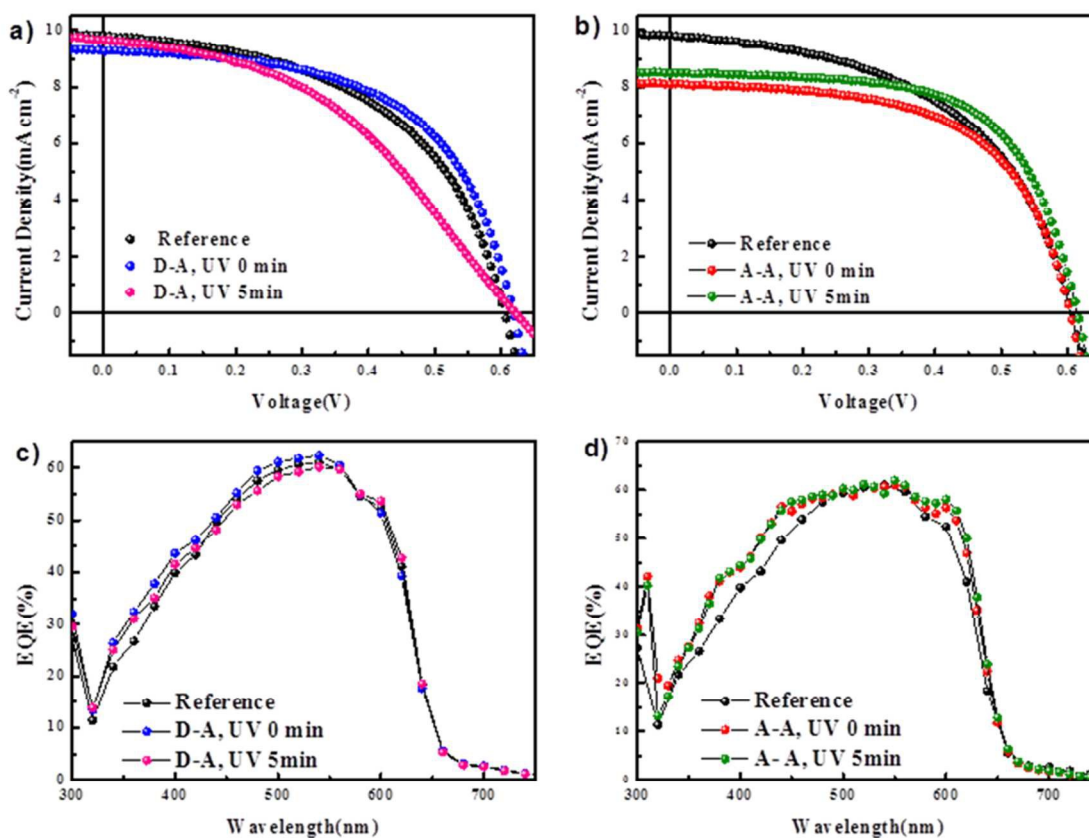


Figure 7. a, b) $J-V$ curves and c, d) EQE spectra of BHJ solar cells with the device structure ITO/ZnO/ active layer/ $\text{MoO}_x(10\text{nm})/\text{Ag}(100\text{nm})$ and ITO/ZnO/polymer/active layer/ $\text{MoO}_x(10\text{nm})/\text{Ag}(100\text{nm})$; a, c) polymer D-A and b, d) polymer A-A.

Table 1. Characteristics, optical and electrochemical properties of the polymers

Polymer	M _w [kg/mol]	PDI	$\lambda_{\max}^{\text{a)}$ [nm]	$\lambda_{\max}^{\text{b)}$ [nm]	$\lambda_{\text{onset}}^{\text{b)}$ [nm]	E _g ^{opt} [eV]	HOMO [eV]	LUMO [eV]
D-A	12.2	1.487	325; 439	326; 448	551	2.25	-5.96	-3.71
A-A	14.0	2.576	509	550	653	1.90	-5.33	-3.43

^{a)}dilute chloroform solutions; ^{b)} thin films spin-cast from chloroform solution.

Table 2. PSC performance parameters of the devices with the structure of ITO/ZnO/ active layer/MoO_x(10nm)/Ag(100nm) and ITO/ZnO/polymer/active layer/MoO_x(10nm)/Ag(100nm).

Material & Conc.	UV irradi. time [min]	V _{oc} [V]	J _{sc} [mA/cm ²]	J _{sc} ^{EQE a)} [mA/cm ²]	FF [%]	PCE ^{b)} [%]
Reference	x	0.61 ± 0.002	8.94 ± 0.559	8.43	50 ± 2.2	2.74 ± 0.181
A-A	0	0.61 ± 0.000	8.15 ± 0.160	8.86	56 ± 2.0	2.78 ± 0.070
4 mg/mL	5	0.61 ± 0.000	8.40 ± 0.130	8.99	60 ± 3.0	3.10 ± 0.160
D-A	0	0.62 ± 0.003	8.90 ± 0.510	8.59	53 ± 2.7	2.91 ± 0.278
2 mg/mL	5	0.62 ± 0.001	8.81 ± 0.530	8.42	41 ± 1.5	2.25 ± 0.016

^{a)} Calculated by integrating the EQE spectrum with the AM1.5G spectrum; ^{b)} the average PCE was obtained from over 8 devices.

GRAPHICAL ABSTRACT

Title: Cross-linkable Polymers Containing Triple Bond Backbone and Their Application in Photovoltaic Devices

Authors: Thi Thu Trang Bui, Sangheon Park, Muhammad Jahandar, Chang Eun Song, Jong-Cheol Lee, Sang Kyu Lee, Sang-Jin Moon, and Won Suk Shin*

Three novel triple bond containing polymers, named A-A, D-A and D-D, were designed and two of them were investigated their photocrosslikability, as well as their application as buffer layers in OPV. The PSC device with A-A polymer buffer layer exhibited the best average PCE of 3.10% after 5 min UV exposure, caused by the improved FF compare to the device with bare ZnO layer. Our research introduced potential candidates for new photocrosslinkable materials which has solvent resistance and hydrophobic nature, and can be used in solution processed multilayer of organic electronic devices

