Simple Structured DPP-based Small Molecules for High Efficient Organic Photovoltaics

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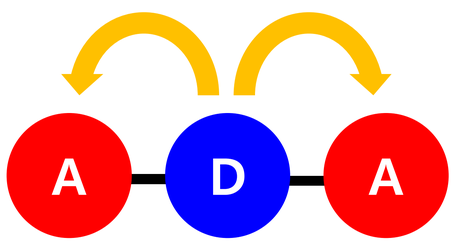
Nanomaterials for Environmentally Friendly Energy Conversion

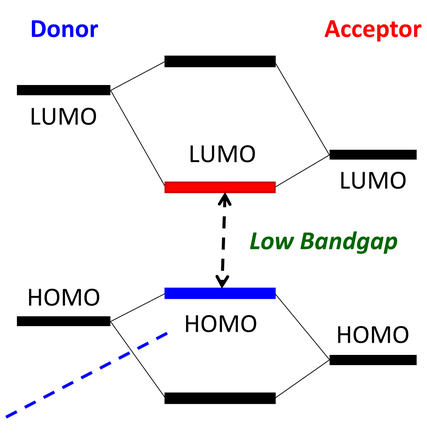
Introduction

▪ **Intramolecular charge transfer**



Donor (D) : electron-rich unit
Acceptor (A) : electron-deficient unit

▪ **Bandgap tuning in D-A type small molecule**



V_{OC} ∝ **HOMO** Energy level of **small molecules**

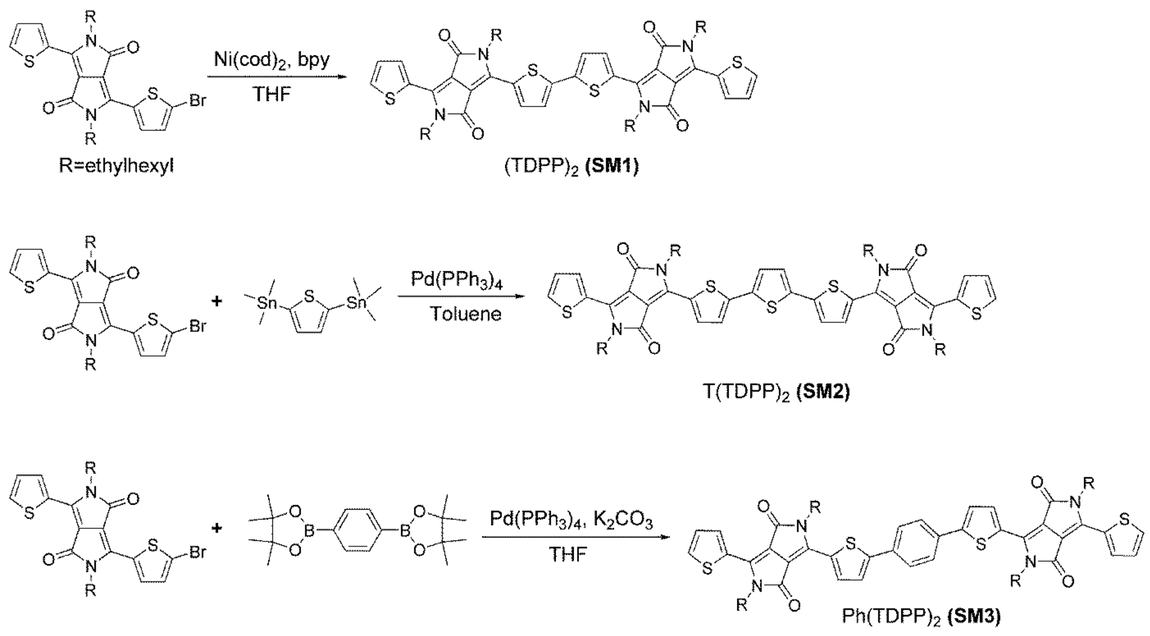
Weak electron-donating power of donor → Deep HOMO energy of small molecule → high V_{OC}

Objectives

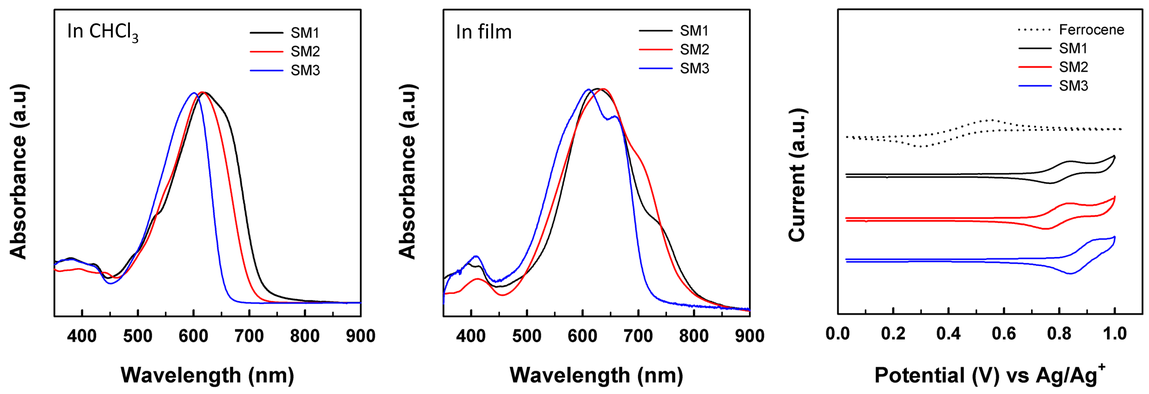
- To synthesize low bandgap small molecules (SM) based on thiophene-capped diketopyrrolopyrrole (TDPP) unit and different electron-donating group with thiophene (T) or phenylene (Ph)
- To precisely control the HOMO energy level by introducing T or Ph
- To investigate the optical, electrochemical, and photovoltaic properties of the SMs

Results

❖ Synthesis



❖ Optical and electrochemical properties

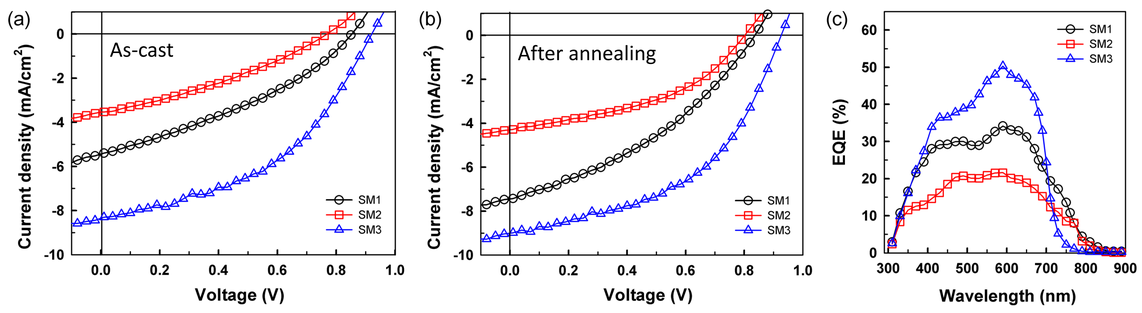


Small molecule	$\lambda_{max, CHCl3}$ (nm)	$\lambda_{max, film}$ (nm)	E_g^{opt} (eV)	HOMO (eV)	LUMO (eV)[a]
SM1	625	628	1.51	-5.18	-3.66
SM2	615	638	1.51	-5.17	-3.68
SM3	601	612	1.66	-5.31	-3.65

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

- **Weak electron-donating** power of Ph → **Deep HOMO** energy level and **large** bandgap of SM1
- **Same electron-deficient** unit → **almost the same LUMO** energy levels of SMs

❖ Photovoltaic properties



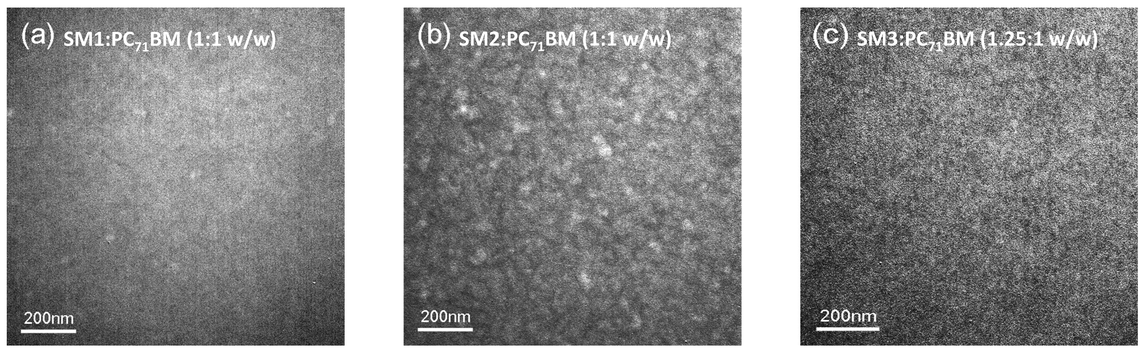
▪ **As-cast**

SMs	SM:$PC_{71}BM$ (w/w)	V_{OC} (V)	J_{SC} (mA/cm²)	FF	PCE (%)
SM1	1:1	0.85	5.41	0.34	1.59
SM2	1:1	0.77	3.60	0.89	0.89
SM3	1.25:1	0.92	8.36	0.45	3.47

▪ **After annealing at 120 ˚C for 10 min.**

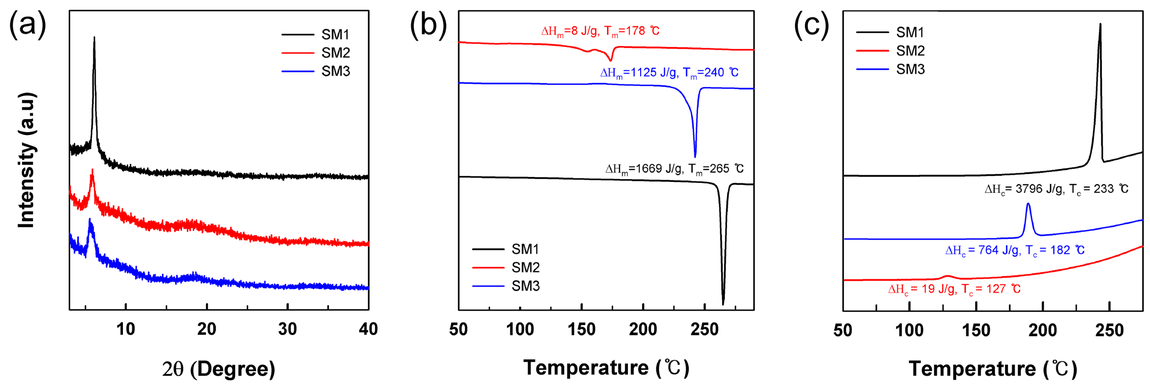
SMs	SM:$PC_{71}BM$ (w/w)	V_{OC} (V)	J_{SC} (mA/cm²)	FF	PCE (%)
SM1	1:1	0.84	7.40	0.37	2.31
SM2	1:1	0.80	4.30	0.43	1.49
SM3	1.25:1	0.93	9.09	0.47	4.01

❖ Morphology study



Homogeneous one-phase morphology | **Macro-phase separated** morphology | **Bicontinuous two-phase nanostructured** morphology

❖ Structure study



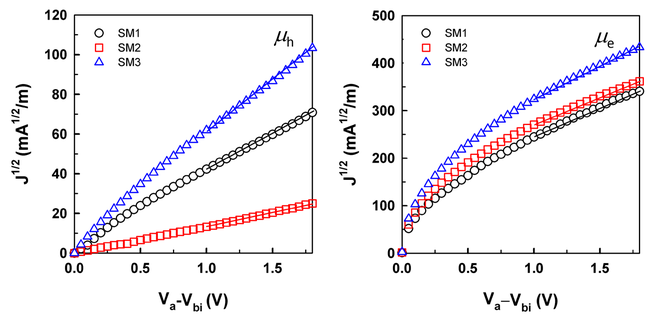
- Strong X-ray diffraction peak at **2θ = 6.10°** for all SMs → (100) diffraction with **14.4 Å** interlayer spacing
- The highest crystallinity of SM1 from XRD (a) and DSC (b, c) data

- **The length scale** of phase separation

  (a): exciton recombination before reaching the D/A interface **(b):** blocking of efficient charge transport

  (c): optimum for charge separation and transport

- **Charge carrier mobility** of SMs (SCLC)



SMs	SM:$PC_{71}BM$ (w/w)	μ_h (cm²/V s)	μ_e (cm²/V s)
SM1	1:1	6.0×10^{-5}	2.2×10^{-4}
SM2	1:1	2.5×10^{-5}	2.0×10^{-4}
SM3	1.25:1	8.8×10^{-5}	2.4×10^{-4}

- **Nano-scale** phase separation of **SM3** → high hole mobility → high J_{SC}

Conclusions

- TDPP-based Small molecules $(TDPP)_2$, $T(TDPP)_2$ and $Ph(TDPP)_2$ are successfully synthesized and show ***V_{OC}* of 0.84 V, 0.80 V and 0.93 V,** respectively.
- $Ph(TDPP)_2$ shows the best PCE of **4.01 %** with a high V_{OC} of **0.93 V** and a high J_{SC} of **9.09 mA/cm²**.