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Supplementary information for

Synthesis and Characterization of Cyano-substituted Pyridine Derivatives for Applications as Exciton Blocker in Photovoltaic Device

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1. Thermal properties measurements

TGA measurements were performed on a TA Instrument TGAQ50 with a heating rate of 10 ^{o}C min^{-1} under a nitrogen atmosphere. *T*g and melting phase-transition temperature (*T*m) were determined by DSC performed on a TA Instrument DSC2910. The sample was firstly heated at a rate of 10 ^{o}C min^{-1} to melt and then quenched, in which process *T*m was obtained. The quenched samples were heated for a second time at a rate of 10 ^{o}C min^{-1}, and then *T*g was recorded.

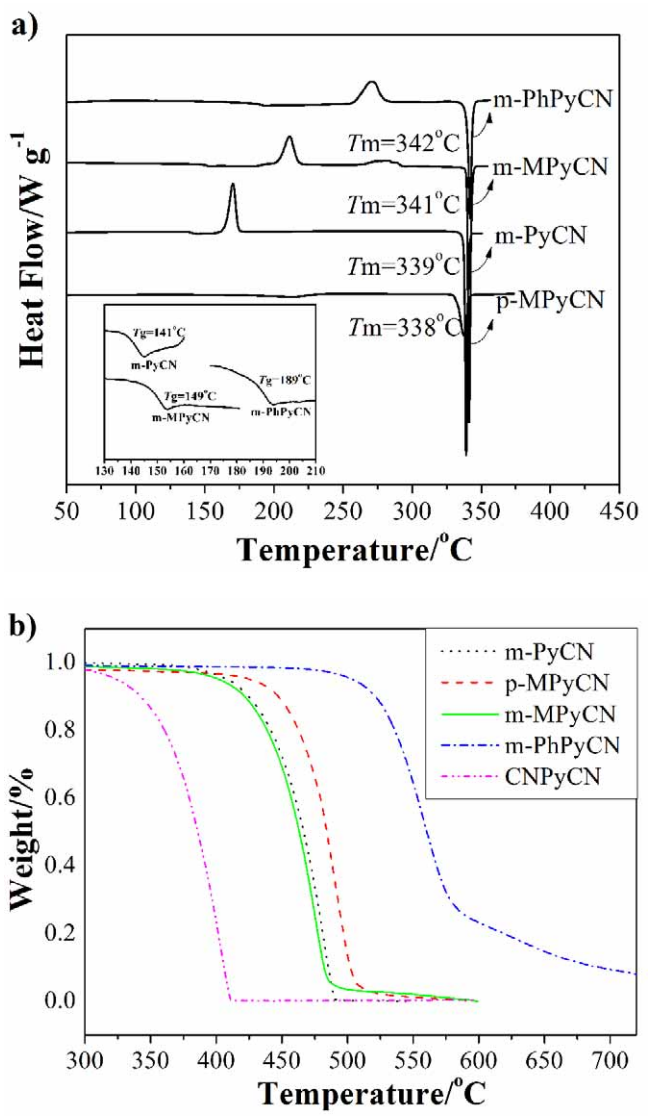


Figure S1. a): DSC data of the cyano-substituted pyridine derivatives. b): TGA data of the cyano-substituted pyridine derivatives.

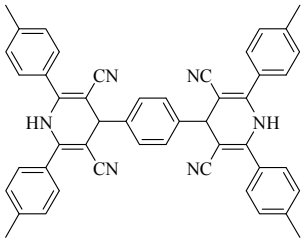
2. Electron mobility measurements

To measure electron mobilities, bilayer electroluminescence (EL) devices with a configuration of ITO/NPB (60 nm)/Materials to be measured (60 nm)/Al (150 nm) were fabricated. Using a pulse generator as an electrical switch in a high-current driver circuit, voltage pulses of 3-12 V with a rise time less than 20 ns was obtained. The devices were driven by voltage pulses with duration of 2-25 μs. EL from the device was detected by a silicon photo-diode attached to a high-speed receiver. The resulting transient photocurrent was analyzed with a storage oscilloscope (HP 54810A). For the interpretation of the luminance delay time, a voltage supply source was employed to give a trigger signal to start the collection of photocurrent. The transient responses of EL of all the devices were measured by averaging the data taken from 100 consecutive signals averaging.

Table S1. Electron mobilities of the cyano-substituted pyridine derivatives and referenced materials measured by transient electroluminescence (EL) method.

Materials	Electron mobility [$cm^2 V^{-1} s^{-1}$]	Electric field [$V cm^{-1}$]	Reference
m-PhPyCN	$4.8\times10^{-5} \sim 5.6\times10^{-5}$	$5.0\times10^{5} \sim 10\times10^{5}$	This work
p-PPTNT	$4.5\times10^{-5} \sim 5.6\times10^{-5}$	$5.0\times10^{5} \sim 10\times10^{5}$	This work
m-MPyCN	$5.6\times10^{-5} \sim 6.1\times10^{-5}$	$5.0\times10^{5} \sim 10\times10^{5}$	This work
p-MPyCN	$3.4\times10^{-5} \sim 3.8\times10^{-5}$	$5.0\times10^{5} \sim 10\times10^{5}$	This work
m-PyCN	$2.9\times10^{-5} \sim 3.3\times10^{-5}$	$5.0\times10^{5} \sim 10\times10^{5}$	This work
CNPyCN	n.a.	n.a.	This work
BCP	6.0×10^{-7}	7.0×10^{5}	Ref [S1]

3. Molecular structure of p-MPyCN's intermediate product.



Scheme S1. Molecular structure of p-MPyCN's intermediate product.

^{1}H NMR (400 MHz, DMSO-d_6, δ): 10.11 (s, 2H), 7.56 (d, 12H, J = 8.0), 7.32 (d, 8H, J = 8.0), 4.72 (s, 2H), 2.37 (s, 12H). MS (EI, m/z): $[M-4]^+$ calcd. for $C_{48}H_{36}N_6$: 696.3; found: 692.3.

S1 Z. Y. Xie, T. C. Wong, L. S. Hung, S. T. Lee, *Appl. Phys. Lett.,* 2002, **80**, 1477.