Supporting information

Exploiting Perylene and Naphthalene Diimides Based Planar Aromatic n-Type Dopants for SWCNT Cathodes in Inverted Perovskite Solar Cells

*Achmad Syarif Hidayat[1], Naoki Ueoka[1], Hisayoshi Oshima[2], Yoshimasa Hijikata[3], and Yutaka Matsuo*1,2*

[1] Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, Nagoya, Aichi, Japan.

[2] Institute of Materials Innovation, Institutes of Innovation for Future Society, Nagoya University, Nagoya, Aichi, Japan.

[3] Advanced Research and Innovation Center, DENSO CORPORATION, Kariya, Aichi, Japan.

*Corresponding author: Yutaka Matsuo: matsuo.yutaka@material.nagoya-u.ac.jp

Experimental

Synthesis and characteristics of SWCNT film

SWCNT films were synthesized using a floating-catalyst chemical vapor deposition (FCCVD) method, resulting in intertwined structure, high purity, and extended nanotube bundle lengths. The synthesis process occurred at 950 ℃ within a quartz tube reactor with a 50 mm diameter. Cartridges containing ferrocene ($FeCp_2$) as a catalyst precursor and sulfur (S) powder as a catalyst promoter were heated to 30 ℃ and 60 ℃, respectively. Vaporization of the precursor and promoter was facilitated by purging nitrogen (N_2) gas into the cartridges, with subsequent delivery into the reactor. Methane (CH_4) gas serves as the carbon source. To prevent CH_4 polymerization at elevated temperatures and to ensure uniform and stable growth of SWCNT, controlled amounts of CH_4 and hydrogen (H_2) gas were continuously supplied into the reactor. As the reaction proceeded, SWCNT was collected downstream of the reactor by filtration through a mixed cellulose esters membrane filter (Merck Millipore Ltd., RAWP09025). Transparency and sheet resistance were controlled by adjusting the collection time, with SWCNT exhibiting 35% transparency utilized consistently throughout all experiments. The SWCNT films exhibited a sheet resistance of ~80 Ω/sq. The size and quality of SWCNT film were analyzed by Raman spectroscopy (Fig. A).[1] The calculated SWCNT diameters utilized in this study ranged from 1.7 to 1.4 nm with I_D/I_G ratio of 0.007. The Raman spectra showed typical semiconducting SWCNT spectra.[2]

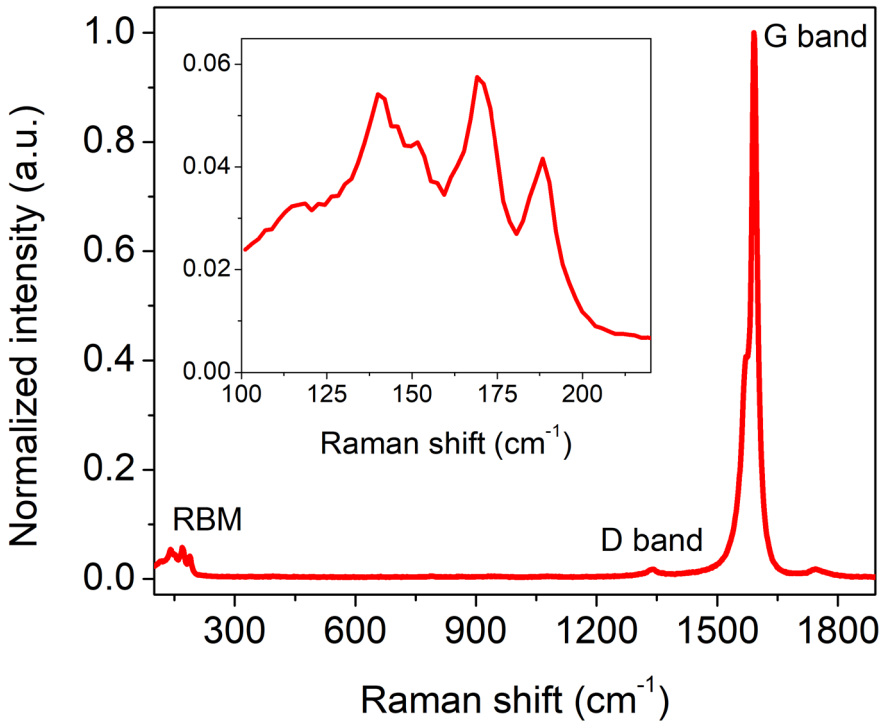


Figure A. The Raman spectrum of the SWCNT film, RBM modes (100 – 200 cm^{-1}) shown in the inset.

Synthesis of $PDINBr_2$

$PDINBr_2$ was synthesized following the procedure reported in the previous work.[3] In a typical reaction, 0.525 g of dibromo-perylene tetracarboxylic dianhydride (TCI) was dissolved in a mixture of 5 mL anhydrous dioxane (Sigma Aldrich) and 5 mL anhydrous N,N-dimethylacetamide (Sigma Aldrich). To this solution, 0.25 mL of N,N-dimethylaminopropylamine was added (Sigma Aldrich). The reaction mixture was refluxed for 6 hours under a nitrogen atmosphere. After completion, the reaction was quenched by the addition of water. The crude product was washed thoroughly with a large amount of water and collected by filtration. The solid was then dried overnight in a vacuum oven, yielding 0.512 g of the desired product. ^{1}H NMR (400 MHz, δ 9.50 (2H, d, *J*=8 Hz); δ 8.93 (2H, s); δ 8.72 (2H, d, *J*=8 Hz); δ 4.28 (4H, t, *J*=7 Hz); δ 2.46 (4H, t, *J*=7 Hz); δ 2.26 (12H, s); δ 1.96 (4H, p, *J*=7 Hz) (Fig. B).

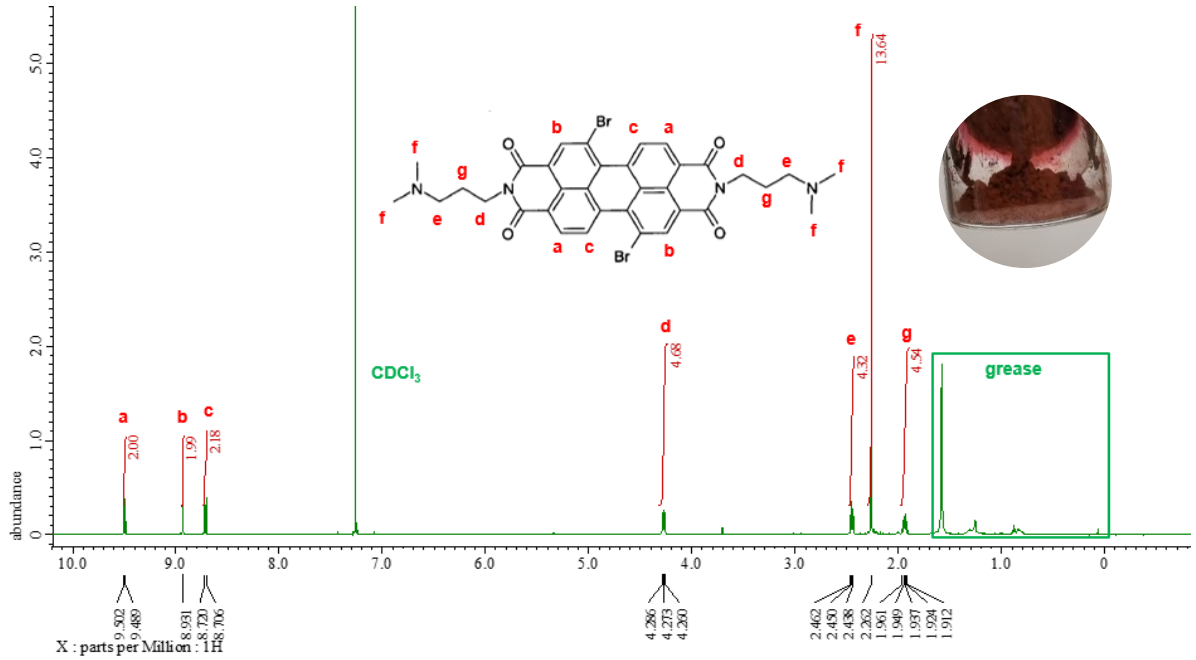


Figure B. The ^{1}H NMR spectra of $PDINBr_2$.

Synthesis of NDIN

NDIN was synthesized by reacting 0.5 g of naphthalene tetracarboxylic dianhydride with 0.9 mL of N,N-dimethylaminopropylamine (TCI) in 15 mL of anhydrous N,N-dimethylformamide (Wako). The reaction mixture was stirred under a nitrogen atmosphere at 140 °C for 18 hours. After completion, the mixture was washed three times with water, saturated NaCl solution, and chloroform. Residual water in the organic phase was removed using anhydrous sodium sulfate (Na_2SO_4). The chloroform was then evaporated, and the resulting solid was collected and dried overnight in a vacuum oven, yielding 0.57 g of the desired product. ^{1}H NMR (400 MHz, δ 8.75 (4H, s); δ 4.27 (4H, t, *J*=7 Hz); δ 2.44 (4H, t, *J*=7 Hz); δ 2.22 (12H, s); δ 1.94 (4H, p, *J*=7 Hz) (Fig. C).

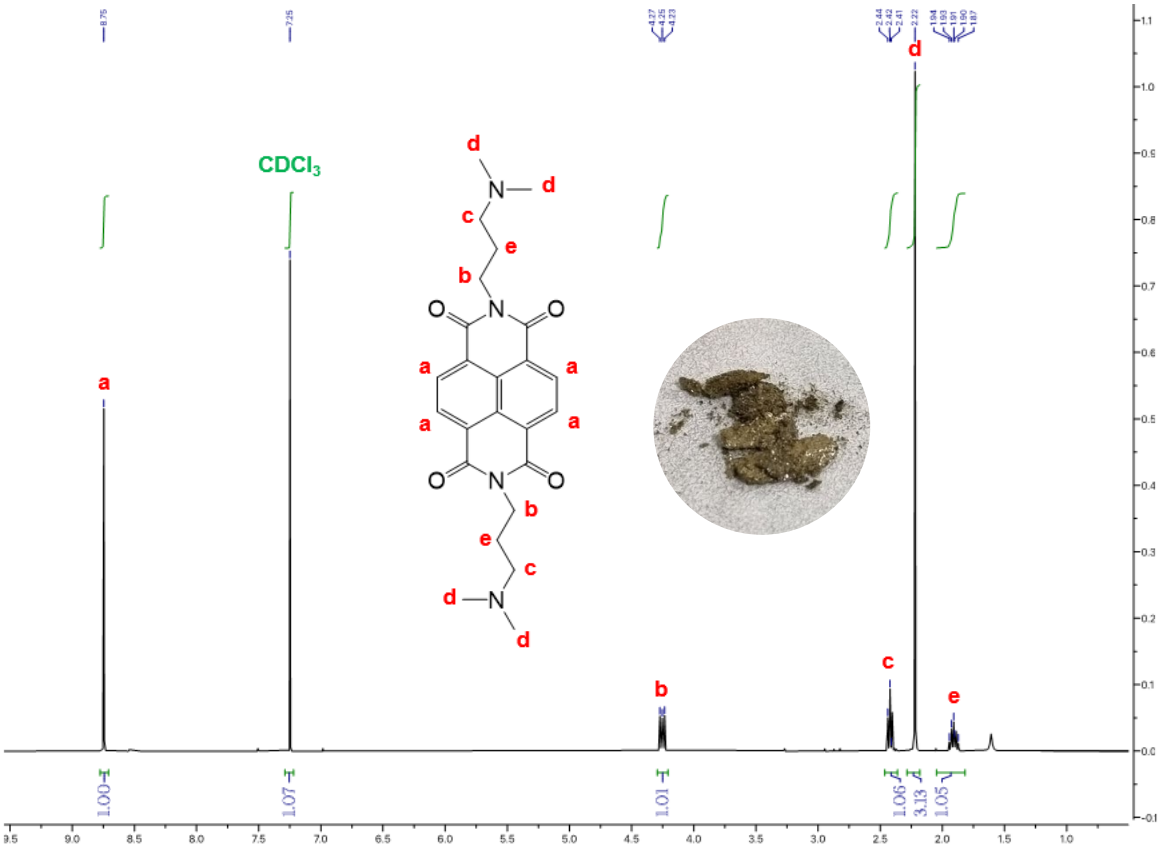


Figure C. The ^{1}H NMR spectra of NDIN.

Perovskite solar cell fabrication

Procedure to fabricate the PSC device are briefly summarized in Fig. D. Glass/ITO substrates with a size of 15 × 15 mm^2 and a sheet resistance of 10 Ω/sq (Techno Print Co., Ltd.) were exposed to UV/O_3 for 30 min., to remove any remaining organic impurities. Poly(3,4 ethylenedioxythiophene) : poly(styrene sulfonate) (PEDOT:PSS) (Clevios P VP, Heraeus Precious Metals GmbH & Co.) layer was fabricated by filtering the PEDOT:PSS solution through 0.2 µm syringe filter (Advantec, DISMIC JP020AN) and spin-coated at 3000 rpm for 20 s, following by heating at 115 ℃ for 10 min. $MAPbI_3$ perovskite layers were fabricated inside a glovebox. Mixture of 355 mg PbI_2 (TCI) and 122 mg MAI (Sigma Aldrich) was dissolved in 490 µL *N,N*-dimethylformamide (DMF). Then, 55 µL of dimethyl sulfoxide (DMSO) (Wako) was added into the solution mixture. The fully dissolved solution was spin-coated onto the PEDOT:PSS layer at 4000 rpm for 20 s, with a dripping of 150 µL of chlorobenzene (CB) (Sigma Aldrich) using 1000 µL micropipette 7 s after starting the spin-coating process. Then, the substrate was heated at 100 ℃ for 10 min, turning brownish transparent film into dark brown film, indicating formation of the $MAPbI_3$ layer. Then, a solution containing 30 mg/mL of PCBM (Frontier Carbon Corporation) in CB was spin coated at 4000 rpm for 20s. SWCNT films were carefully press-transferred onto the PCBM layer inside a glovebox. Simultaneously, N-type doping of the SWCNT films were performed using commercially available PDIN 2.5 wt% (TCI) and synthesized $PDINBr_2$ and NDIN 1 wt% dissolved in 2,2,2-trifluoroethanol (TFE) inside a glovebox. For the reference device (SWCNT

undoped), the TFE solution was spin-coated directly onto the SWCNT films without any dopants. Finally, 100 nm of Ag was vacuum-deposited on the edges, assisting contact during *J–V* measurements.

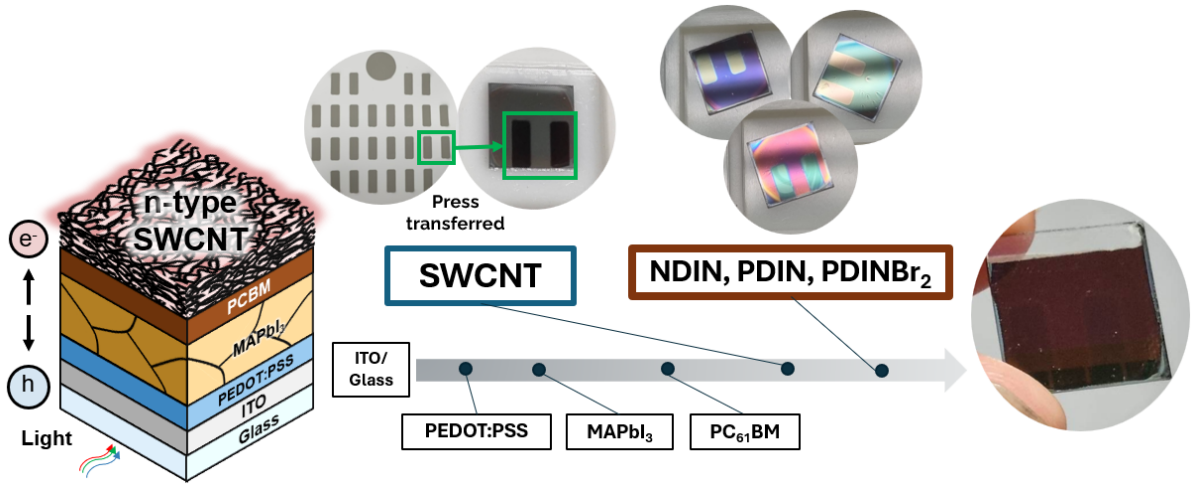


Figure D. Perovskite solar cell fabrication process.

Characterization

^{1}H Nuclear Magnetic Resonance (NMR) spectra were taken by ECS 400 (JEOL Co., Ltd.) at room temperature reported in parts per million (ppm). The spectra were internally referenced to tetramethylsilane (0.00 ppm) or $CDCl_3$ (7.260 ppm). *J–V* characteristics were measured with a software-controlled source meter (Keithley 2400) with a scan rate of 50 mV s^{-1} under 1 sun AM 1.5G simulated sunlight irradiation (100 mW cm^{-2}). The solar simulator (HAL-320W, Asahi Spectra) used a 300 W Xe lamp, and sunlight irradiance was calibrated with a silicon pyranometer (EKO ML-01). All measurements were conducted using a 0.04 cm^2 mask placed on the PSC active area. Scanning electron microscopy (SEM) observations were performed using JSM-7000F (JEOL), while energy-dispersive X-ray spectroscopy (EDS) observation was performed using S-4800 (Hitachi High-Tech Co.). Atomic force microscopy observation was carried out with NX20 AFM (PARK). Work function was measured with a photoemission yield spectroscopy in air (PYSA) in air (AC-2, Riken Keiki). Raman spectra were taken using confocal Raman microscope system (Renishaw, inVia reflex), using a 532 nm excitation laser and 1800 l/mm grating. Near infrared (NIR) absorption spectra were taken using ARCoptix FT-NIR *Rocket*. X-ray photoelectron spectroscopy (XPS) spectra were acquired using VG scientific ESCALAB250. Microwave photoconductivity decay spectra were obtained at $\lambda_{ex.}$ = 349 nm, $\lambda_{meas.}$ = 26 GHz (KOBELCO LTA-1512EP). Sheet resistance measurement was performed using a four-point probe system. *S* measurement system (ZEM-2, Advance Riko) was used to evaluate doping characteristics of SWCNT. For the *S* measurement, samples were placed inside a helium-filled chamber. Then, temperature gradient was performed across the sample by heating the substrate on one side at 130 °C, and controlling the temperature different steady at 10 °C, 15 °C, and 20 °C on the other side. Two K-type thermocouple probes were placed in the middle part of SWCNT film and placed 0.6 cm apart from each other. Temperature difference (ΔT) and voltage difference (ΔV) were simultaneously measured using the probes for each temperature gradients, then *S* value was calculated using the equation: $S = -\frac{\Delta V}{\Delta T}$. The

electron mobility (μ) was determined by fitting the dark current of ITO/SWCNT/Ag device to Mott-Gurney equation [4,5], which is described by the equation: $I = \frac{9}{8}\varepsilon_r\varepsilon_0 A_{eff}\mu\frac{V^2}{L^3}$,where ε_0 = 8.85 × 10^{-14} F/cm is the free space permittivity, ε_r = 3 is dielectric constant, L = 100 nm is the film thickness, estimated from cross sectional SEM imaging, and A_{eff} = 0.09 cm^2 is the effective film area. The lifetime decay was fit using the equation: $y = A_1 e^{-x/\tau_1} + A_2 e^{-x/\tau_2} + I_0$, where initial rapid decay (τ_1), attributed to the interfacial charge transfer lifetime, followed by a slower subsequent decay (τ_2), associated with the free carrier lifetime within the bulk perovskite.

Computational calculation method

Structural models for PCBM, PDIN, $PDINBr_2$, NDIN, (5,0) SWCNT (diameter ≈ 4.1 Å, length ≈ 35.4 Å), and their respective complexes were optimized using density functional theory (DFT) employing the Becke, 3-parameter, Lee-Yang-Parr hybrid exchange-correlation functional (B3LYP) (Table. S4 – S11). The (5,0) SWCNT was chosen due to its semiconducting nature and small diameter, enabling efficient computational treatment while preserving essential features of electronic interaction. To model the SWCNT realistically, its length was optimized, and a ~3 nm structure was determined to effectively mimic the electronic characteristics of the experimentally used nanotube. To suppress edge effects, the nanotube was passivated with hydrogen atoms at both termini. Geometry optimizations were performed using the 6-31G basis set in the Gaussian 16 Rev. C.01 program package[6]. Based on the optimized structures, adsorption behaviour and electronic properties were further investigated. The charge density difference distribution $\Delta\rho(\mathrm{r})$ was computed using equation (1),

$$\Delta\rho(\mathrm{r}) = \rho(\mathrm{r})_{\mathrm{complex}} - [\rho(\mathrm{r})_{\mathrm{SWCNT}} + \rho(\mathrm{r})_{\mathrm{dopants}}] \qquad (1)$$

Where $\rho(\mathrm{r})_{\mathrm{complex}}$, $\rho(\mathrm{r})_{\mathrm{SWCNT}}$, and $\rho(\mathrm{r})_{\mathrm{dopants}}$ denote the electron densities of the SWCNT–dopant complex, the isolated SWCNT, and the isolated dopant, respectively. All densities were computed at the same geometry as the complex to isolate electronic effects from structural relaxation. Hirshfeld charge analysis was employed to evaluate charge distribution and electron transfer. The atomic charge q_A was calculated according to equation (2) [7],

$$q_A = Z_A - \int \frac{\rho_A^0(\mathrm{r})}{\sum_B \rho_B^0(\mathrm{r})}\rho(\mathrm{r})\,\mathrm{dr} \qquad (2)$$

where Z_A is the nuclear charge of atom A, $\rho(\mathrm{r})$ is the molecular electron density, and $\rho_A^0(r)$ and $\rho_B^0(r)$ represent the pro-atomic reference densities of atoms A and B, respectively, in their neutral states. Further analyses, including molecular orbital visualization, total and partial density of states (DOS), and population analysis, were conducted using the Multiwfn wavefunction analysis program[8]. Single-point energy calculations were employed for $\Delta\rho(\mathrm{r})$ mapping, ensuring consistent geometries between pristine and doped systems. The Hirshfeld

method was selected for its robustness in capturing localized electron accumulation and depletion due to molecular doping. From the Hirshfeld charges, the total charge on the SWCNT sidewall for both the doped ($\sum q_{\mathrm{doped}}$) and pristine ($\sum q_{\mathrm{pristine}}$) systems were determined. The transferred charge (Δq) was then derived as the absolute difference between these two values, using equation (3).

$$\Delta q = \left|\sum q_{\mathrm{doped}} - \sum q_{\mathrm{pristine}}\right| \qquad (3)$$

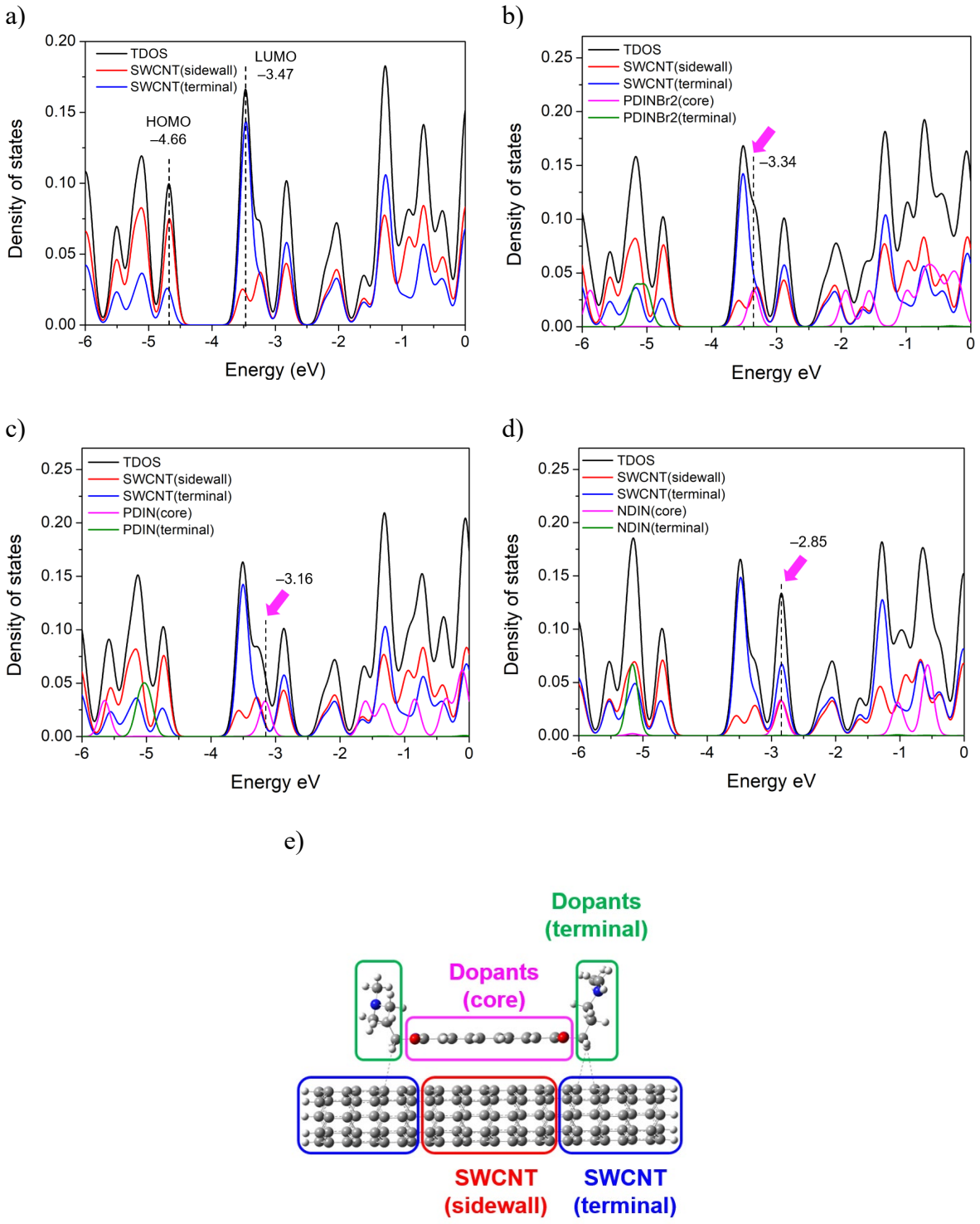


Figure S1. Partial density of states (PDOS) of (a) the pristine SWCNT, (b–d) SWCNT–dopant complexes, with the decomposition based on (c) the corresponding structural fragmentation.

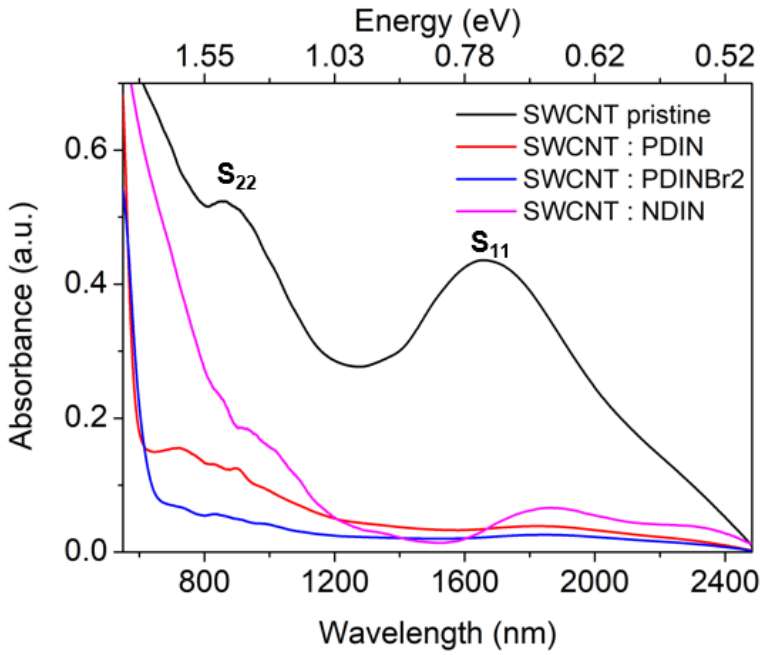


Figure S2. Near-infrared (NIR) absorption spectra of pristine and n-doped SWCNT films.

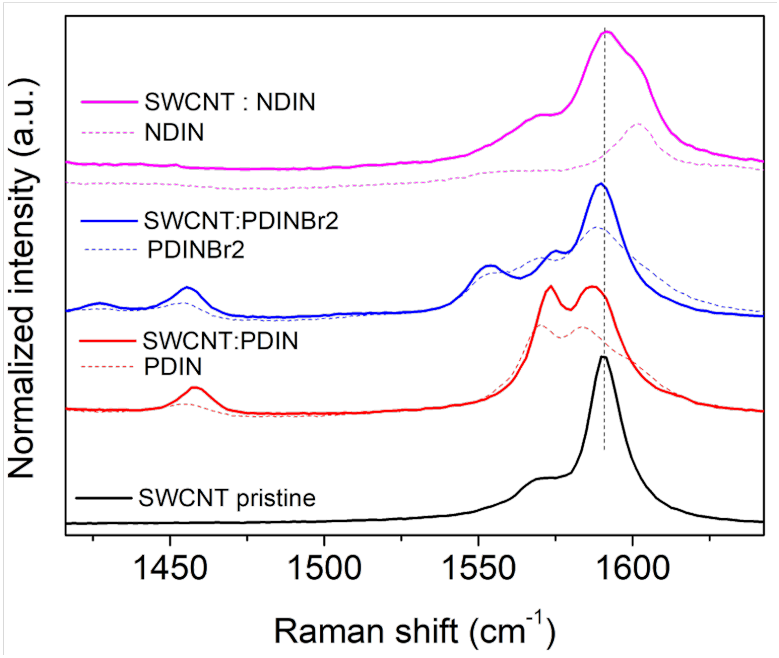


Figure S3. Raman spectra of pristine and n-doped SWCNT films compared to their corresponding dopants.

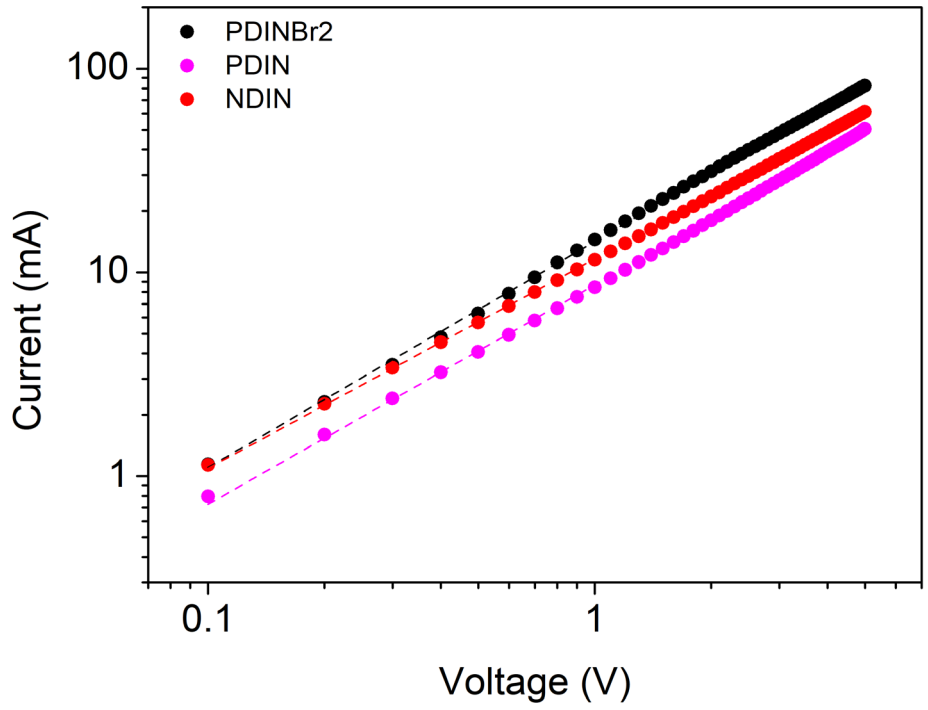


Figure S4. Dark log(*I*)–log(*V*) characteristics of ITO/SWCNT:dopant/Ag device. The trap-free SCLC region were fitted and their intercept was used to calculate the carrier mobility (μ).[9]

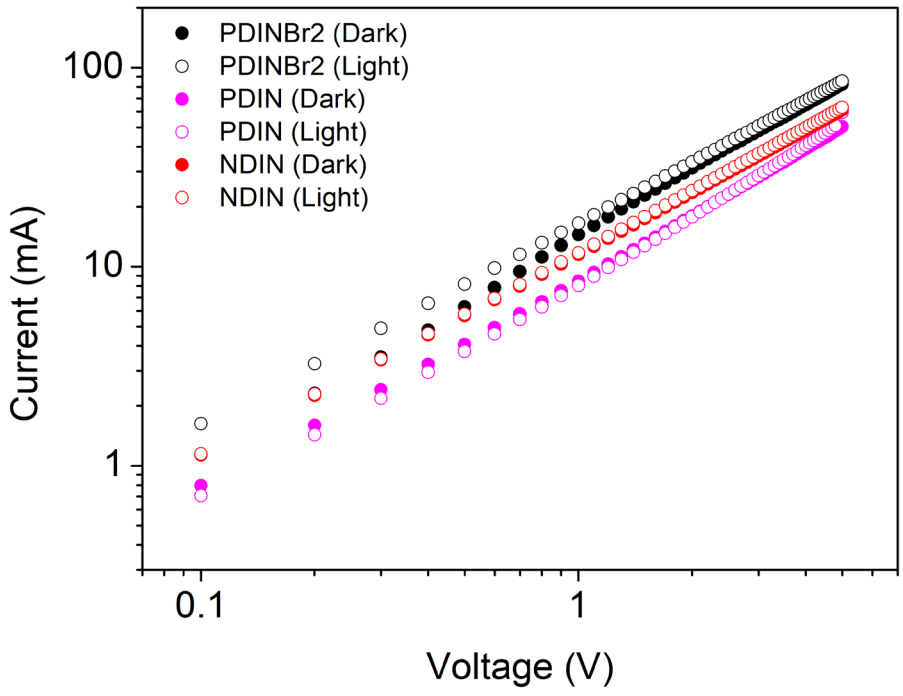


Figure S5. Dark current-voltage (*I–V*) plot of pristine and doped SWCNT films (with PDIN, $PDINBr_2$, and NDIN) measured under dark and illuminated (1 sun) conditions.

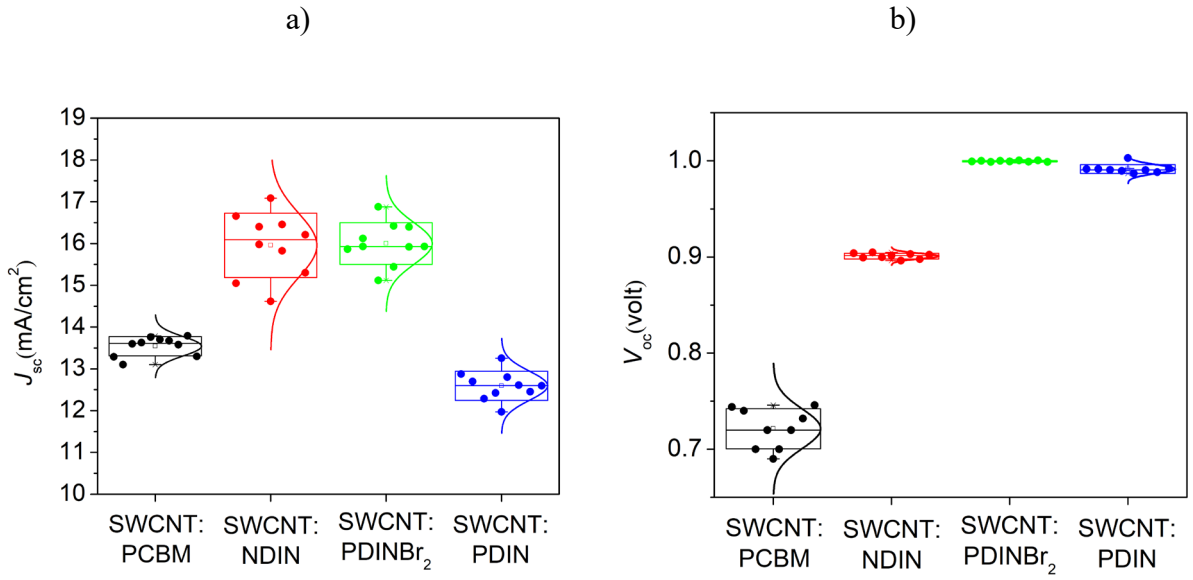
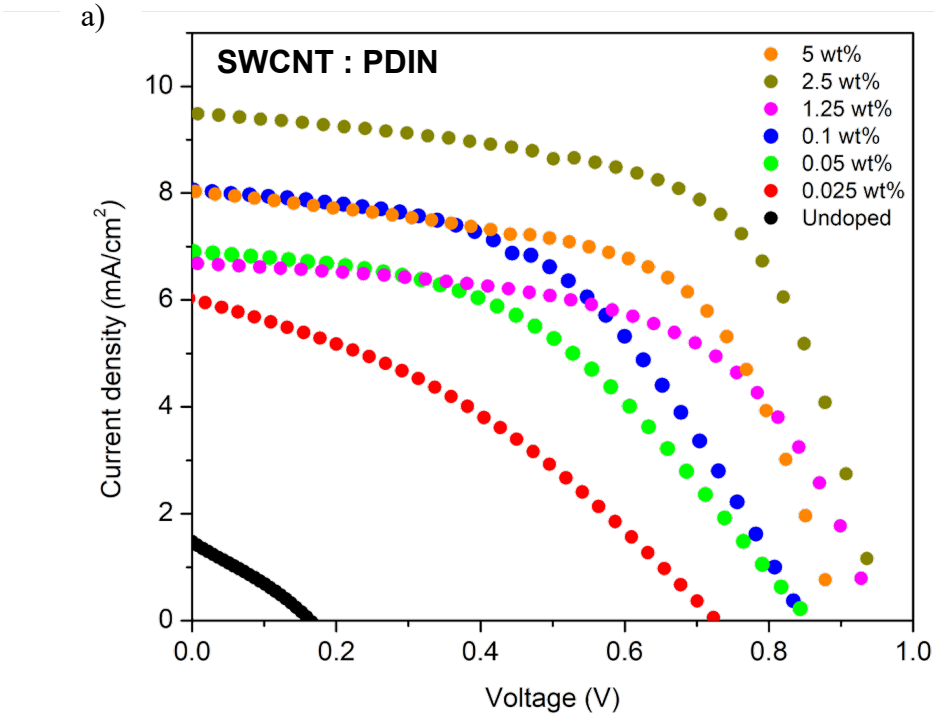


Figure S6. PSC device statistical distributions of (a) short-circuit current density, and (b) open-circuit voltage compared among dopants (n = 10).



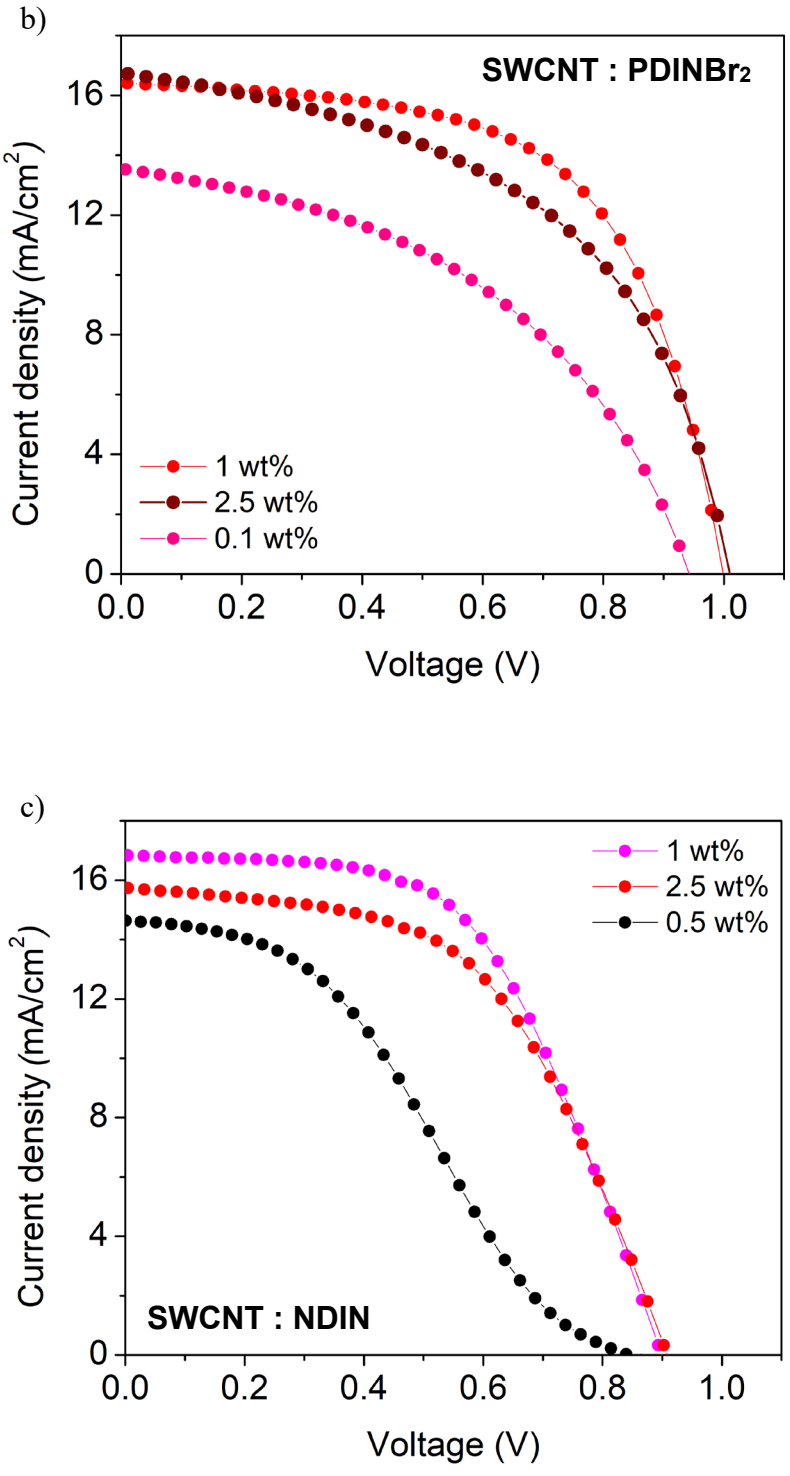


Figure S7. *J–V* characteristics of PSCs employing (a) PDIN, (b) $PDINBr_2$, and (c) NDIN-doped SWCNT cathodes with different dopant concentrations.

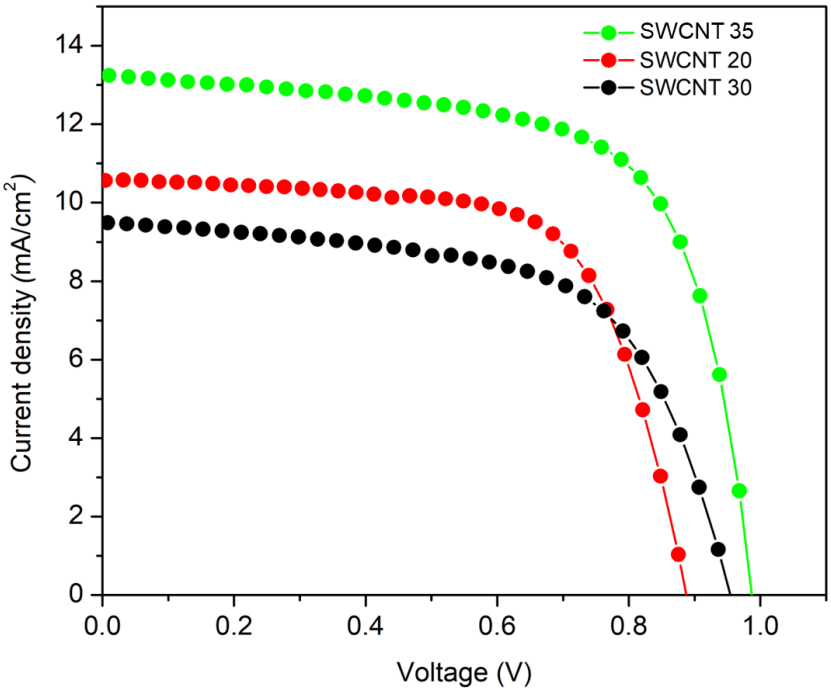


Figure S8. *J–V* characteristics of PSCs employing PDIN-doped SWCNT cathodes with different SWCNT transmittance (T) = 35%, 30%, and 20%.

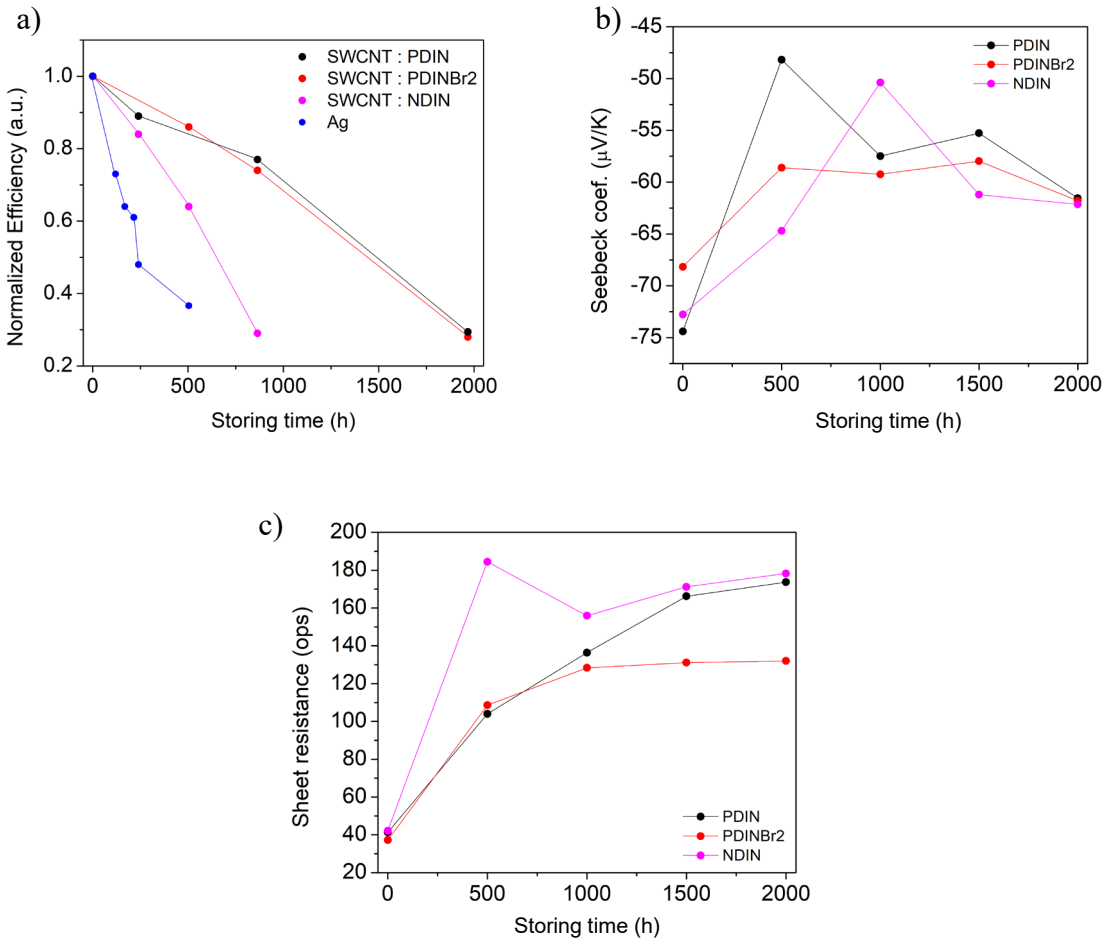


Figure S9. Long-term stability assessment of inverted PSCs using doped SWCNT electrodes (a) Normalized PCE, (b) *S*, and (c) R_{Sheet} of doped SWCNT films.

Table S1. Total charge (Σq) and transferred charge (Δq) in electrons (e) on the SWCNT sidewall parallel to the dopant core. Σq represents the absolute Hirshfeld charge on this region, while Δq is the difference between the pristine and doped states.

Method	$\Sigma q_{SWCNT|core}$ (e)				Δq $_{pristine - doped}$ (e)		
	Pristine	$PDINBr_2$ doped	PDIN doped	NDIN doped	$PDINBr_2$ doped	PDIN doped	NDIN doped
Hirshfield charge	–0 .3306	–0.4237	–0.4194	–0.3425	0.0932	0.0888	0.0119
Atomic dipole corrected Hirshfield charge (ADCH)	–0.3145	–0.4100	–0.4074	–0.3402	0.0955	0.0929	0.0257

Table S2. Electrical properties of inverted PSCs utilizing pristine (control), PDIN, $PDINBr_2$, and NDIN-doped SWCNT cathodes with different dopant concentrations.

Dopants	Doping conc. (wt%)	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	R_s ($\Omega \cdot cm^2$)	R_{sh} ($\Omega \cdot cm^2$)	η (%)
Control	SWCNT Ref.	1.48	0.16	0.28	51.51	134.72	0.07
PDIN	0.025	6.01	0.73	0.35	73.65	262.32	1.52
	0.05	6.90	0.86	0.45	60.26	954.72	2.65
	0.1	10.42	0.87	0.41	44.01	778.19	3.78
	1.25	6.68	0.95	0.57	22.19	1298.71	3.63
	2.5	9.49	0.95	0.62	14.83	868.26	5.57
	5	8.03	0.89	0.59	19.28	626.71	4.24
$PDINBr_2$	2.5	16.74	1.01	0.51	10.67	322.48	8.55
	1	16.87	1.00	0.63	8.20	947.49	10.12
	0.1	13.54	0.94	0.45	17.61	311.43	5.75
NDIN	0.5	14.63	0.84	0.35	28.22	675.9	4.43
	1	16.84	0.89	0.55	17.62	1740.7	8.38
	2.5	15.74	0.90	0.53	18.54	632.4	7.64

Table S3. Exponential fitting results ($I_0 = 0$) of μ-PCD data.

Sample	$\boldsymbol{A_1}$	τ_1 (ns)	$\boldsymbol{A_2}$	τ_2 (ns)
ITO/PVK/PCBM/SWCNT:$PDINBr_2$	0.34	83.05	0.55	667.37
ITO/PVK/PCBM/ SWCNT:PDIN	0.36	89.41	0.52	676.34
ITO/PVK/PCBM/ SWCNT:NDIN	0.44	74.71	0.42	574.12

Table S4. Cartesian coordinate from optimized structure of PDIN.

XYZ coordinates of PDIN		
C 1.25951 2.75996 0.10329	H -0.73609 -2.92970 -1.83571	C -5.16252 1.19412 -0.60324
C 0.60870 1.58800 -0.30029	H -3.19310 -3.05150 -1.95207	O -5.53470 -2.20590 -1.75185

C 1.40348 0.44653 -0.65016	C 5.11238 -0.49324 -0.83969	O -5.89584 2.16282 -0.30354
C 2.83002 0.54054 -0.57324	C 4.91399 1.85978 -0.07547	N -5.71831 -0.02626 -1.02267
C 3.44418 1.74993 -0.15689	O 5.84239 -1.46113 -1.15072	C -7.19934 -0.13211 -1.12238
C 2.65623 2.84331 0.17450	O 5.48459 2.91924 0.26809	C -7.85256 -0.84062 0.07664
H 0.68628 3.63756 0.37198	N 5.66873 0.72069 -0.40106	C -7.70069 -0.08863 1.40810
C 0.80702 -0.78585 -1.07704	C 7.15116 0.83907 -0.32629	N -8.52165 -0.67375 2.48411
C 3.63936 -0.57361 -0.91593	C 7.69435 0.80414 1.11618	C -8.71894 0.24347 3.61279
H 3.14325 3.75915 0.48832	C 7.50256 -0.51025 1.90102	C -8.08276 -2.00421 2.92103
C 3.04070 -1.75618 -1.32803	N 8.66995 -1.41319 1.85736	H -6.63015 -0.04184 1.69885
C 1.64559 -1.85749 -1.40609	H 7.54692 0.02619 -0.93224	H -8.02850 0.94737 1.26907
H 3.67407 -2.59655 -1.58664	H 7.41288 1.79669 -0.78288	H -8.92502 -0.93730 -0.13658
C -3.09090 2.46062 -0.12410	H 8.76830 1.02917 1.08517	H -7.44785 -1.85630 0.14389
C -3.68954 1.27720 -0.53340	H 7.22381 1.62762 1.66413	H -7.57263 0.88776 -1.22274
C -2.88060 0.16290 -0.87730	H 7.34909 -0.26265 2.95820	H -7.41088 -0.69298 -2.03472
C -1.45397 0.25756 -0.80227	H 6.57906 -1.02352 1.56323	H -9.13662 1.18824 3.25130
C -0.85739 1.49058 -0.37716	C 8.56102 -2.50343 2.83362	H -7.78376 0.46974 4.16477
C -1.69567 2.56253 -0.04852	C 9.03058 -1.89774 0.51668	H -9.42940 -0.19636 4.32053
H -3.72431 3.30083 0.13508	H 8.40350 -2.08704 3.83431	H -8.78490 -2.39027 3.66685
C -3.49463 -1.04597 -1.29622	H 9.49337 -3.07726 2.84596	H -7.06963 -1.99889 3.37432
C -0.65899 -0.88287 -1.15523	H 7.73015 -3.20668 2.62029	H -8.07406 -2.70063 2.07898
C -1.30953 -2.05341 -1.56318	H 8.21622 -2.45524 0.01879	H 1.22465 -2.79958 -1.73210
C -2.70628 -2.13710 -1.63379	H 9.90325 -2.55343 0.60031	H -1.27449 3.50503 0.27592
C -4.96456 -1.15607 -1.37933	H 9.31239 -1.05933 -0.12603	

Table S5. Cartesian coordinate from optimized structure of $PDINBr_2$.

XYZ coordinates of $PDINBr_2$		
C 1.29503 2.65491 -0.90868	H -3.17941 -3.25177 -1.84532	C -5.15079 1.04921 -0.67623
C 0.63038 1.44210 -0.68652	C 5.10937 -0.74734 -0.57421	O -5.52600 -2.37126 -1.74836
C 1.40783 0.23226 -0.67826	C 4.93804 1.69936 -0.93454	O -5.87488 2.03427 -0.41398
C 2.83406 0.33784 -0.70196	O 5.82047 -1.76734 -0.44069	N -5.70860 -0.17342 -1.07733
C 3.46567 1.59410 -0.88009	O 5.51877 2.78801 -1.13609	C -7.18799 -0.26605 -1.21694
C 2.68910 2.73192 -1.02320	N 5.68177 0.52149 -0.74959	C -7.88263 -0.93782 -0.02024
H 0.73084 3.56844 -0.98178	C 7.16638 0.63400 -0.80030	C -7.76153 -0.15449 1.29634
C 0.78308 -1.06769 -0.63764	C 7.77615 1.24418 0.47738	N -8.61918 -0.70543 2.36117
C 3.63217 -0.82341 -0.55701	C 7.62405 0.43004 1.77924	C -8.84407 0.24212 3.45946
H 3.17698 3.68281 -1.20075	N 8.79101 -0.41530 2.09946	C -8.20476 -2.02755 2.84514
C 3.02328 -2.04881 -0.36992	H 7.53618 -0.37194 -0.98997	H -6.69931 -0.11038 1.61698
C 1.62715 -2.16465 -0.40338	H 7.40262 1.27695 -1.65163	H -8.07495 0.88074 1.12252
H 3.64147 -2.92255 -0.21031	H 8.84698 1.40926 0.30172	H -8.94935 -1.02877 -0.26245
C -3.08050 2.29988 -0.18931	H 7.33123 2.23582 0.61336	H -7.49173 -1.95579 0.08404
C -3.67639 1.11738 -0.58147	H 7.51758 1.13149 2.61525	H -7.54666 0.75494 -1.35302
C -2.86947 -0.01368 -0.85824	H 6.68759 -0.16407 1.74929	H -7.37894 -0.84657 -2.12148
C -1.44608 0.08205 -0.75445	C 8.73218 -0.94250 3.46793	H -9.24301 1.18014 3.06117
C -0.82794 1.36016 -0.49721	C 9.09096 -1.46065 1.10990	H -7.92476 0.47576 4.03430
C -1.68462 2.41435 -0.14329	H 8.61991 -0.11502 4.17656	H -9.57958 -0.17441 4.15551

H -3.70799 3.14285 0.06911	H 9.66647 -1.46449 3.69857	H -8.93217 -2.38861 3.57907
C -3.48862 -1.22924 -1.24369	H 7.89527 -1.65135 3.63296	H -7.20574 -2.01819 3.32848
C -0.66513 -1.11661 -0.90190	H 8.25649 -2.16880 0.95414	H -8.17697 -2.74587 2.02207
C -1.31558 -2.28265 -1.32527	H 9.96863 -2.02304 1.44406	Br 1.03621 -3.99080 -0.02690
C -2.70287 -2.33762 -1.51218	H 9.34022 -1.00938 0.14565	Br -1.11559 4.16349 0.52161
H -0.74602 -3.17824 -1.50315	C -4.95685 -1.32096 -1.37974	

Table S6. Cartesian coordinate from optimized structure of NDIN.

XYZ coordinates of NDIN		
C 2.99911 -0.95528 -1.02883	O -3.75135 1.95457 -1.04685	H -5.58077 1.33311 0.97992
C 1.52453 -1.09028 -1.02186	O -3.30646 -2.63990 -0.97543	H -5.96397 0.24440 2.32471
C 0.70817 0.07006 -1.01885	O 3.75124 -1.95299 -1.04988	C 4.99685 0.50240 -0.97255
C 1.28230 1.36737 -1.01855	O 3.30636 2.64138 -0.97181	C 5.52716 0.75591 0.45029
C 2.75461 1.51873 -1.00850	C -4.99694 -0.50091 -0.97321	C 5.29386 -0.38950 1.45094
C 0.93924 -2.35044 -1.02834	C -5.52723 -0.75652 0.44926	N 3.88861 -0.52894 1.89158
C -0.70828 -0.06851 -1.01891	C -5.29370 0.38737 1.45160	C 3.44953 0.53548 2.80388
C -1.28239 -1.36583 -1.02047	N -3.88840 0.52599 1.89231	C 3.59478 -1.87076 2.41621
C -0.46372 -2.48844 -1.02516	C -3.44945 -0.53975 2.80310	H 4.00689 0.53647 3.76241
C -2.75470 -1.51719 -1.01052	C -3.59432 1.86703 2.41877	H 3.57626 1.51636 2.33813
C -2.99920 0.95684 -1.02732	H -4.00661 -0.54183 3.76175	H 2.38630 0.40559 3.02979
C -1.52463 1.09183 -1.02018	H -3.57660 -1.51997 2.33608	H 4.17075 -2.11691 3.33048
H 1.58284 -3.22200 -1.03629	H -2.38613 -0.41052 3.02899	H 3.82154 -2.61606 1.64875
H -0.92591 -3.46853 -1.02692	H -4.17013 2.11198 3.33346	H 2.52976 -1.94062 2.66116
C 0.46362 2.48999 -1.02155	H -3.82108 2.61344 1.65239	H 6.61189 0.91049 0.36090
C -0.93934 2.35200 -1.02485	H -2.52925 1.93640 2.66368	H 5.11586 1.69888 0.82627
H 0.92581 3.47008 -1.02190	H -5.42133 0.41610 -1.38357	H 5.58100 -1.33451 0.97784
H -1.58293 3.22357 -1.03152	H -5.25669 -1.34439 -1.61591	H 5.96420 -0.24774 2.32420
N -3.52281 -0.34657 -1.04106	H -6.61198 -0.91082 0.35969	H 5.42126 -0.41400 -1.38425
N 3.52272 0.34814 -1.04064	H -5.11602 -1.70010 0.82378	H 5.25660 1.34683 -1.61400

Table S7. Cartesian coordinate from optimized structure of SWCNT [5,0].

XYZ coordinates of SWCNT [5,0]		
C -13.11387 -1.45334 -1.37513	C -6.01287 2.05093 0.26767	C 8.86000 -0.37590 -2.01630
C -12.41373 -0.37631 -2.01836	C -6.73665 1.81028 -0.98461	C 8.13619 0.88941 -1.86845
C -13.11362 0.86004 -1.80575	C -3.88921 1.81315 -0.98543	C 6.01286 -2.05093 -0.26767
C -12.41335 -2.04002 -0.26620	C -1.76505 0.88379 -1.85476	C 8.86033 -2.03768 -0.26593
C -13.11380 -1.75940 0.95678	C -2.48613 -0.37706 -2.01880	C 8.13613 -1.81988 0.99003
C -12.41374 -0.88303 1.85485	C -1.76445 -1.49725 -1.41551	C 6.73665 -1.81028 0.98461
C -13.11376 0.36648 1.96496	C -0.36106 -1.49698 -1.41512	C 6.01307 -0.88687 1.86265
C -12.41355 1.49252 1.41262	C 0.36032 -0.37698 -2.01767	C 8.86001 -0.88194 1.85285
C -13.11388 1.98649 0.25900	C -0.36038 0.88352 -1.85401	C 6.73630 0.37708 2.02171
C -12.41341 1.80692 -0.98292	C -2.48712 -2.04742 -0.26715	C 8.13620 0.37914 2.03323
C -10.26302 0.88884 -1.86740	C 0.36144 -2.04815 -0.26725	C 6.01293 1.50018 1.41953

C -10.98696 -0.37152 -1.99256	C -0.36106 -1.81180 0.98409	C 8.86024 1.49091 1.41126
C -10.26297 -1.50237 -1.42219	C -1.76443 -1.81215 0.98441	C 8.13617 2.05484 0.26816
C -8.86024 -1.49091 -1.41126	C -2.48616 -0.88385 1.85508	C 6.73681 2.04432 0.26676
C -8.13620 -0.37913 -2.03323	C 0.36038 -0.88352 1.85400	C 6.01293 1.81589 -0.98749
C -8.86002 0.88194 -1.85285	C -1.76509 0.37707 2.01849	C 8.86027 1.80476 -0.98185
C -10.98713 -2.01400 -0.26277	C -0.36032 0.37699 2.01767	C 10.98705 0.87174 -1.83108
C -8.13617 -2.05484 -0.26816	C -2.48680 1.49675 1.41528	C 10.26312 -0.37883 -2.03206
C -8.86027 -1.80476 0.98185	C 0.36106 1.49698 1.41511	C 10.98716 -1.47346 -1.39458
C -10.26299 -1.81870 0.98948	C -0.36143 2.04815 0.26725	C 12.41355 -1.49252 -1.41261
C -10.98704 -0.87174 1.83108	C -1.76414 2.04837 0.26729	C 13.11376 -0.36648 -1.96495
C -8.13619 -0.88941 1.86845	C -2.48681 1.81158 -0.98428	C 12.41374 0.88302 -1.85484
C -10.26312 0.37883 2.03206	C 0.36107 1.81181 -0.98410	C 10.26294 -2.05332 -0.26796
C -8.86000 0.37590 2.01630	C 2.48617 0.88386 -1.85509	C 13.11388 -1.98649 -0.25899
C -10.98716 1.47346 1.39459	C 1.76509 -0.37706 -2.01849	C 12.41341 -1.80692 0.98292
C -8.13615 1.50342 1.42313	C 2.48680 -1.49675 -1.41529	C 10.98706 -1.78378 0.97033
C -8.86034 2.03768 0.26593	C 3.88923 -1.49800 -1.41685	C 10.26302 -0.88885 1.86740
C -10.26294 2.05332 0.26797	C 4.61167 -0.37710 -2.02073	C 13.11362 -0.86004 1.80577
C -10.98707 1.78377 -0.97032	C 3.88957 0.88491 -1.85775	C 10.98696 0.37152 1.99257
C -8.13614 1.81988 -0.99003	C 1.76414 -2.04837 -0.26729	C 12.41373 0.37631 2.01837
C -6.01308 0.88687 -1.86265	C 4.61245 -2.04621 -0.26704	C 10.26297 1.50237 1.42219
C -6.73630 -0.37708 -2.02171	C 3.88921 -1.81315 0.98543	C 13.11387 1.45333 1.37514
C -6.01293 -1.50018 -1.41953	C 2.48681 -1.81158 0.98428	C 12.41336 2.04002 0.26620
C -4.61220 -1.49644 -1.41561	C 1.76505 -0.88379 1.85476	C 10.98713 2.01400 0.26277
C -3.88963 -0.37744 -2.02165	C 4.61171 -0.88432 1.85683	C 10.26299 1.81870 -0.98947
C -4.61172 0.88432 -1.85684	C 2.48613 0.37706 2.01880	C 13.11381 1.75939 -0.95677
C -6.73681 -2.04432 -0.26677	C 3.88963 0.37744 2.02165	H 14.19643 -0.89226 1.87359
C -3.88903 -2.04879 -0.26734	C 1.76445 1.49725 1.41550	H 14.19658 1.50855 1.42748
C -4.61220 -1.81130 0.98468	C 4.61220 1.49644 1.41561	H 14.19649 1.82669 -0.99342
C -6.01293 -1.81588 0.98749	C 3.88903 2.04879 0.26733	H 14.19651 -2.06301 -0.26898
C -6.73636 -0.88449 1.85783	C 2.48712 2.04742 0.26715	H 14.19659 -0.38029 -2.03846
C -3.88957 -0.88491 1.85774	C 1.76443 1.81216 -0.98442	H -14.19644 0.89226 -1.87358
C -6.01313 0.37812 2.02702	C 4.61220 1.81130 -0.98469	H -14.19658 -1.50855 -1.42747
C -4.61167 0.37711 2.02073	C 6.73636 0.88449 -1.85783	H -14.19651 2.06301 0.26899
C -6.73666 1.49553 1.41542	C 6.01313 -0.37812 -2.02702	H -14.19648 -1.82670 0.99343
C -3.88923 1.49800 1.41685	C 6.73667 -1.49553 -1.41542	H -14.19659 0.38029 2.03848
C -4.61245 2.04621 0.26704	C 8.13615 -1.50342 -1.42313	

Table S8. Cartesian coordinate from optimized complex structure of PDIN SWCNT [5,0].

XYZ coordinates of PDIN SWCNT [5,0]		
C -13.11920 0.15187 -0.38409	C 1.77606 0.09690 0.63524	C -1.37590 4.14581 0.10645
C -12.39876 0.17347 0.85902	C 2.47882 0.12003 -0.65021	C -2.80732 4.15325 0.09048
C -13.08841 -0.61960 1.83787	C 3.87999 0.11431 -0.67294	C -3.53459 4.14356 1.30860
C -12.43956 -0.52839 -1.45204	C 4.62340 0.08242 0.59074	C -2.85233 4.12303 2.51701
C -13.15315 -1.72606 -1.79809	C 3.91320 -0.68605 1.61393	H -0.96329 4.09312 3.50728
C -12.45589 -2.94436 -1.49202	C 1.73597 -0.61011 -1.67910	C -0.66349 4.15387 -1.13786

C -13.14394 -3.65503 -0.45019	C 4.58262 -0.62563 -1.72427	C -3.50807 4.16529 -1.14340
C -12.42390 -3.73669 0.79026	C 3.84752 -1.82515 -2.12626	H -3.42484 4.11028 3.43699
C -13.10370 -2.97163 1.79896	C 2.44447 -1.81777 -2.10148	C -2.79779 4.16893 -2.33609
C -12.38901 -1.80704 2.24341	C 1.72210 -3.03084 -1.71952	C -1.39723 4.16445 -2.32993
C -10.23695 -0.59850 1.84837	C 4.56961 -3.04663 -1.76627	H -3.34912 4.17298 -3.26891
C -10.97283 0.13981 0.82775	C 2.45594 -3.80259 -0.71697	H -0.88726 4.16393 -3.28429
C -10.26846 0.19953 -0.44910	C 3.85909 -3.81161 -0.74005	C 2.91338 4.07842 2.58113
C -8.86634 0.17574 -0.46678	C 1.75401 -3.82643 0.56636	C 3.62359 4.09726 1.38867
C -8.12200 0.16308 0.79692	C 4.60187 -3.84029 0.52083	C 2.92333 4.12347 0.15451
C -8.83428 -0.61626 1.81294	C 3.89899 -3.10903 1.57792	C 1.49187 4.13081 0.13862
C -11.01323 -0.55337 -1.45342	C 2.49734 -3.10102 1.59869	C 0.77934 4.11355 1.38286
C -8.16324 -0.54700 -1.53068	C 1.78801 -1.89172 2.01834	C 1.51280 4.08714 2.57487
C -8.90077 -1.75249 -1.91794	C 4.63466 -1.90604 1.97480	H 3.46469 4.05462 3.51371
C -10.30379 -1.74338 -1.91185	C 6.75897 -0.70049 1.56924	C 3.65050 4.14048 -1.06391
C -11.02878 -2.93820 -1.49312	C 6.02375 0.07998 0.57038	C 0.80753 4.15004 -1.12142
C -8.17880 -2.98039 -1.57341	C 6.72730 0.09527 -0.71690	H 1.00256 4.06793 3.52889
C -10.29413 -3.73702 -0.51843	C 8.12639 0.09850 -0.74231	C 1.56756 4.16465 -2.29700
C -8.89103 -3.73068 -0.53562	C 8.87041 0.05203 0.52070	C 2.96799 4.16067 -2.27210
C -10.99786 -3.72035 0.75987	C 8.15893 -0.70119 1.55646	H 1.07871 4.17599 -3.26229
C -8.14715 -3.77701 0.72610	C 5.98333 -0.62976 -1.75077	H 3.54036 4.16888 -3.19221
C -8.85023 -3.02942 1.77301	C 8.83007 -0.65086 -1.78759	C -4.98396 4.17316 -1.17693
C -10.25247 -3.03048 1.80827	C 8.09337 -1.84676 -2.20495	C -5.00993 4.14779 1.30521
C -10.96296 -1.81559 2.19391	C 6.69396 -1.84004 -2.17097	O -5.62098 4.18341 -2.25478
C -8.11189 -1.83364 2.18970	C 5.97020 -3.05712 -1.79355	O -5.68047 4.13023 2.36227
C -5.98800 -0.62799 1.77535	C 8.81738 -3.06403 -1.82881	N -5.65553 4.17576 0.05786
C -6.72275 0.14412 0.77085	C 6.70605 -3.82449 -0.78525	C -7.14276 4.13580 0.05857
C -6.01919 0.17278 -0.51649	C 8.10568 -3.84160 -0.81105	C -7.79190 5.48483 0.42612
C -4.61938 0.16018 -0.53746	C 6.00269 -3.85212 0.49999	C -7.56944 6.65579 -0.55309
C -3.87594 0.13034 0.72597	C 8.84984 -3.85432 0.45133	N -8.66006 6.83857 -1.53377
C -4.58663 -0.63978 1.74804	C 8.14595 -3.13464 1.51715	H -7.43270 3.79864 -0.93487
C -6.76379 -0.56179 -1.54405	C 6.74682 -3.12110 1.53033	H -7.43487 3.38447 0.79589
C -3.91731 -0.57719 -1.59072	C 6.03580 -1.91300 1.95849	H -8.87366 5.32996 0.53281
C -4.65323 -1.77758 -1.99004	C 8.88218 -1.92711 1.90277	H -7.42223 5.76580 1.41819
C -6.05438 -1.76916 -1.97370	C 11.00849 -0.73837 1.47805	H -7.52247 7.58684 0.02474
C -6.77917 -2.98232 -1.58604	C 10.27304 0.06006 0.50365	H -6.58710 6.54856 -1.05548
C -3.93204 -3.00008 -1.63188	C 10.97691 0.04321 -0.77489	C -8.54022 8.11003 -2.25671
C -6.04432 -3.75935 -0.58436	C 12.40283 0.06155 -0.80525	C -8.87373 5.70069 -2.44142
C -4.64297 -3.76262 -0.60462	C 13.12284 -0.01844 0.43541	H -8.49171 8.93737 -1.54048
C -6.74764 -3.77553 0.70083	C 12.43556 -0.73010 1.47713	H -9.42290 8.25642 -2.88817
C -3.90023 -3.79553 0.65647	C 10.23241 -0.64823 -1.82262	H -7.64291 8.16670 -2.90637
C -4.60269 -3.06084 1.71171	C 13.08372 -0.70248 -1.81374	H -7.98136 5.44519 -3.04064
C -6.00263 -3.05541 1.73826	C 12.37051 -1.86800 -2.25852	H -9.69690 5.94152 -3.12231
C -6.71249 -1.84233 2.15567	C 10.94445 -1.86156 -2.20908	H -9.16659 4.81392 -1.87308
C -3.86605 -1.85973 2.11097	C 10.21996 -3.08021 -1.86439	C 5.12601 4.13190 -1.06132
C -1.74116 -0.65740 1.70104	C 13.07140 -3.05450 -1.85319	C 5.09933 4.09094 1.42154
C -2.47417 0.12011 0.70275	C 10.95672 -3.81690 -0.84294	O 5.79724 4.15103 -2.11787

C -1.77141 0.14424 -0.58295	C 12.38282 -3.84857 -0.87414	O 5.74064 4.08113 2.49659
C -0.36950 0.13624 -0.60525	C 10.25247 -3.87639 0.43361	N 5.76946 4.10445 0.18657
C 0.37335 0.10420 0.65734	C 13.10325 -3.82529 0.36886	C 7.25517 4.04887 0.18829
C -0.33605 -0.66566 1.67818	C 12.42282 -3.14606 1.43683	C 7.92881 5.41472 -0.02745
C -2.51465 -0.58648 -1.61155	C 10.99639 -3.12319 1.43826	C 7.67308 6.42433 1.10204
C 0.33216 -0.60262 -1.65655	C 10.28522 -1.93411 1.89673	N 8.51135 7.63325 0.98308
C -0.40224 -1.80208 -2.05541	C 13.13460 -1.94704 1.78312	C 8.57794 8.40171 2.23161
C -1.80661 -1.79413 -2.03361	H 14.15290 -3.10270 -1.93173	C 8.18383 8.48023 -0.16989
C -2.52935 -3.00709 -1.65207	H 14.18579 -3.90375 0.37390	H 6.59518 6.68567 1.14143
C 0.31827 -3.02279 -1.69659	H 14.21843 -1.95362 1.84142	H 7.91080 5.95116 2.06098
C -1.79574 -3.77922 -0.64931	H 14.16544 -0.66111 -1.89258	H 9.01200 5.24712 -0.09245
C -0.39144 -3.78664 -0.67135	H 14.20608 0.04914 0.44333	H 7.60776 5.81089 -0.99692
C -2.49765 -3.80240 0.63378	H -14.16978 -0.56965 1.91673	H 7.54351 3.61977 1.14866
C 0.35047 -3.81853 0.58859	H -14.20146 0.23354 -0.38967	H 7.54192 3.36903 -0.61603
C -0.35153 -3.08589 1.64402	H -14.18552 -3.01129 1.87762	H 8.91360 7.75248 3.04627
C -1.75407 -3.07823 1.66667	H -14.23696 -1.71777 -1.85634	H 7.60589 8.84752 2.52656
C -2.46304 -1.86816 2.08615	H -14.22740 -3.71959 -0.45747	H 9.30190 9.21620 2.12140
C 0.38369 -1.88424 2.04013	C -1.45194 4.11337 2.54203	H 8.89372 9.31222 -0.22176
C 2.50947 -0.68031 1.63412	C -0.69170 4.12423 1.36647	H 7.16013 8.90587 -0.11777
H 8.26701 7.91085 -1.09878		

Table S9. Cartesian coordinate from optimized complex structure of $PDINBr_2$ SWCNT [5,0].

XYZ coordinates of $PDINBr_2$ SWCNT [5,0]		
C 12.61149 -3.62332 -1.98664	C -2.28496 -3.98849 -1.00064	C 3.86213 3.55557 2.38182
C 11.88517 -4.52027 -1.13159	C -2.98033 -3.05997 -1.89234	C 4.52201 3.61034 1.16978
C 12.59107 -4.69368 0.10794	C -4.38212 -3.00655 -1.88120	C 3.78547 3.84878 -0.01673
C 11.95553 -2.36894 -2.23006	C -5.13085 -3.87845 -0.97440	C 2.36518 4.00567 0.04427
C 12.70197 -1.30094 -1.62378	C -4.40456 -4.10914 0.27577	C 1.67045 3.79288 1.29050
C 12.03492 -0.66008 -0.52428	C -2.21283 -1.83247 -2.09770	C 2.46575 3.65325 2.43834
C 12.73711 -0.93558 0.69849	C -5.05719 -1.72227 -2.07256	H 4.43878 3.42098 3.28747
C 12.01409 -1.75942 1.62719	C -4.28595 -0.61361 -1.50810	C 4.47020 3.92220 -1.25574
C 12.66839 -3.03040 1.76774	C -2.88473 -0.66922 -1.52049	C 1.66432 4.38606 -1.15223
C 11.92102 -4.14498 1.25462	C -2.12922 -0.11418 -0.39452	C 2.37427 4.39915 -2.35959
C 9.73961 -4.65371 0.14453	C -4.97538 -0.00454 -0.36694	C 3.75210 4.15435 -2.41713
C 10.46059 -4.44342 -1.10642	C -2.84773 -0.29288 0.87005	H 1.86022 4.61514 -3.28002
C 9.76112 -3.54831 -2.02194	C -4.24916 -0.23709 0.88439	H 4.27560 4.16497 -3.36553
C 8.35950 -3.48835 -1.99438	C -2.15356 -1.22386 1.75763	C -4.10070 4.92949 -0.96725
C 7.61007 -4.37334 -1.09884	C -4.99690 -1.11239 1.78616	C -4.11681 3.65614 1.16026
C 8.33830 -4.58548 0.15509	C -4.32216 -2.39535 1.98490	O -4.73247 5.49205 -1.88954
C 10.53005 -2.31990 -2.19047	C -2.92055 -2.44990 1.96958	O -4.78303 3.10338 2.06230
C 7.68117 -2.20665 -2.20446	C -2.24762 -3.61407 1.39037	N -4.76799 4.31123 0.09974
C 8.45261 -1.10578 -1.62156	C -5.09408 -3.50320 1.41718	C -6.25662 4.28273 0.09032
C 9.85438 -1.14709 -1.64582	C -7.24969 -3.99580 0.30221	C -6.89443 5.25618 1.10109
C 10.60905 -0.63277 -0.50699	C -6.53095 -3.82862 -0.96375	C -6.66478 6.76221 0.85807
C 7.76198 -0.48312 -0.48745	C -7.22736 -2.89550 -1.85380	N -7.75801 7.42814 0.12028

C 9.89097 -0.76821 0.75676	C -8.62600 -2.84615 -1.85106	H -6.55246 4.50452 -0.93338
C 8.48882 -0.72972 0.76262	C -9.37554 -3.70659 -0.93163	H -6.55045 3.26059 0.34078
C 10.58775 -1.71808 1.61694	C -8.64872 -3.95158 0.31702	H -7.97687 5.07388 1.11819
C 7.74031 -1.59281 1.67910	C -6.45758 -1.66693 -2.06519	H -6.52208 4.98701 2.09532
C 8.41798 -2.87905 1.85893	C -9.30194 -1.55810 -2.02877	H -6.60481 7.26508 1.83082
C 9.81995 -2.93397 1.86200	C -8.52888 -0.44308 -1.47462	H -5.68573 6.92183 0.36246
C 10.49633 -4.07279 1.24904	C -7.13090 -0.50498 -1.47985	C -7.63095 8.88987 0.15122
C 7.64635 -3.99559 1.30498	C -6.37403 0.05483 -0.35443	C -7.98862 6.91781 -1.23981
C 5.49252 -4.49032 0.18334	C -9.21997 0.14929 -0.32493	H -7.57084 9.23205 1.18999
C 6.21162 -4.31093 -1.08076	C -7.09350 -0.12858 0.91106	H -8.51596 9.34362 -0.30701
C 5.51390 -3.38676 -1.97858	C -8.49167 -0.06460 0.92924	H -6.73702 9.26750 -0.38598
C 4.11417 -3.33116 -1.95990	C -6.39734 -1.05511 1.80502	H -7.10279 7.00225 -1.89514
C 3.36606 -4.20557 -1.05467	C -9.24178 -0.94924 1.82376	H -8.81383 7.47743 -1.69236
C 4.09246 -4.43256 0.19563	C -8.56531 -2.23136 2.03596	H -8.28661 5.86653 -1.20383
C 6.28244 -2.15568 -2.17976	C -7.16685 -2.28410 2.01085	C 5.93355 3.73728 -1.32327
C 3.43796 -2.04773 -2.15295	C -6.49342 -3.45213 1.43426	C 5.99096 3.45005 1.14023
C 4.20814 -0.94037 -1.58610	C -9.33852 -3.33155 1.45219	O 6.56209 3.77797 -2.40379
C 5.60788 -0.98981 -1.60303	C -11.49590 -3.80064 0.33787	O 6.65881 3.26907 2.18217
C 6.36354 -0.44031 -0.47281	C -10.77798 -3.66604 -0.92553	N 6.61464 3.51615 -0.11462
C 3.51810 -0.32783 -0.44706	C -11.47360 -2.71559 -1.78623	C 8.08535 3.30732 -0.18600
C 5.64458 -0.61021 0.79473	C -12.89993 -2.67182 -1.79623	C 8.89303 4.61102 -0.30186
C 4.24491 -0.56186 0.80501	C -13.62386 -3.49405 -0.86698	C 8.78774 5.52503 0.92875
C 6.34123 -1.54505 1.68196	C -12.92198 -3.77108 0.35543	N 9.75467 6.63885 0.89168
C 3.49736 -1.43766 1.70758	C -10.70382 -1.50083 -2.03161	C 9.94313 7.26922 2.20383
C 4.17322 -2.72006 1.90346	C -13.55220 -1.39944 -1.93741	C 9.49437 7.62590 -0.16317
C 5.57318 -2.77359 1.89633	C -12.80277 -0.28638 -1.42427	H 7.74816 5.89874 1.03672
C 6.24834 -3.93523 1.31011	C -11.37833 -0.36086 -1.41883	H 8.99846 4.93531 1.82755
C 3.40219 -3.83023 1.33839	C -10.62061 0.21954 -0.31429	H 9.94892 4.33903 -0.43122
C 1.24649 -4.32554 0.22245	C -13.47193 0.26304 -0.27735	H 8.58363 5.13276 -1.21402
C 1.96409 -4.15069 -1.04047	C -11.34178 0.00883 0.93669	H 8.36008 2.75617 0.71402
C 1.26847 -3.22269 -1.93185	C -12.76631 0.08796 0.96212	H 8.26747 2.68471 -1.06365
C -0.13453 -3.16887 -1.91798	C -10.64357 -0.88726 1.85153	H 10.22494 6.51010 2.94016
C -0.88197 -4.04227 -1.01367	C -13.49382 -0.80736 1.81753	H 9.03696 7.78898 2.57652
C -0.15650 -4.27159 0.23553	C -12.83971 -2.06275 2.06139	H 10.75202 8.00503 2.14280
C 2.03544 -1.99482 -2.13720	C -11.41427 -2.11418 2.02151	H 10.29201 8.37583 -0.16221
C -0.80899 -1.88648 -2.11025	C -10.74038 -3.28835 1.47682	H 8.52712 8.15410 -0.03289
C -0.03950 -0.77886 -1.54606	C -13.58783 -3.12968 1.45549	H 9.48858 7.14507 -1.14440
C 1.36299 -0.83185 -1.55938	C -0.55303 3.06015 2.22067	Br 0.21219 6.41796 -3.53714
C 2.11810 -0.27599 -0.43380	C 0.20341 3.68985 1.22431	Br 1.80310 3.63542 4.27900
C -0.72883 -0.16775 -0.40759	C -0.48593 4.21839 0.07882	H -14.55076 0.38199 -0.27945
C 1.39977 -0.45351 0.83112	C -1.91570 4.25349 0.09900	H -14.57383 -0.73118 1.89426
C -0.00270 -0.40062 0.84377	C -2.64078 3.65057 1.15694	H -14.67121 -3.14219 1.52030
C 2.09438 -1.38558 1.71836	C -1.95308 3.02384 2.18299	H -14.63431 -1.34530 -2.00227
C -0.74925 -1.27790 1.74397	H -0.05730 2.58954 3.05167	H -14.70872 -3.51878 -0.89078
C -0.07503 -2.55890 1.94109	C 0.23021 4.71170 -1.07225	H 13.67023 -4.80977 0.10996
C 1.32796 -2.61227 1.92847	C -2.62274 4.88376 -0.95410	H 13.69164 -3.69781 -2.06329

C 2.00129 -3.77605 1.35010	H -2.51326 2.51964 2.96070	H 13.75060 -3.08260 1.83256
C -0.84571 -3.66785 1.37679	C -1.92126 5.48596 -1.98049	H 13.78527 -1.28615 -1.68891
C -3.00255 -4.16218 0.26229	C -0.52368 5.40677 -2.03081	H 13.82182 -0.90737 0.72338
H -2.46887 6.00692 -2.75480		

Table S10. Cartesian coordinate from optimized complex structure of NDIN SWCNT [5,0].

XYZ coordinates of NDIN SWCNT [5,0]		
C 13.25033 -0.43676 -1.92631	C 0.58006 -3.39818 0.93438	H -13.98571 -3.87965 -0.15811
C 12.56987 -1.67853 -2.16619	C 1.98360 -3.37323 0.91877	H -14.06111 0.02100 -0.78115
C 13.29663 -2.76014 -1.55956	C 2.69503 -3.56794 -0.34468	H -14.03523 -2.15693 -1.88621
C 12.54346 0.47701 -1.07331	C -0.15221 -3.61979 -0.31247	H 14.37929 -2.79641 -1.62701
C 13.25493 0.64295 0.16445	C -2.30157 -3.08523 -1.42555	H 14.33171 -0.38411 -2.00400
C 12.57631 0.11128 1.31454	C -1.60555 -1.93566 -2.00763	H 14.41329 -3.16355 0.78544
C 13.30349 -1.01638 1.82809	C -2.34631 -0.69412 -1.79466	H 14.33597 0.73971 0.16437
C 12.62475 -2.27510 1.69103	C -3.75084 -0.71764 -1.78173	H 14.38665 -0.98465 1.89036
C 13.32912 -3.11613 0.76364	C -4.45269 -1.98573 -1.97666	C -3.23962 4.19999 -1.62525
C 12.61917 -3.38392 -0.45610	C -3.70277 -3.11081 -1.41068	C -1.77832 4.24480 -1.39184
C 10.44630 -2.85881 -1.57540	C -1.63220 0.22522 -0.91254	C -1.27585 4.32380 -0.06758
C 11.14372 -1.69998 -2.12378	C -4.47822 0.17537 -0.88210	C -2.15398 4.36192 1.04578
C 10.39927 -0.45695 -1.95508	C -3.74498 0.40354 0.36721	C -3.61719 4.32959 0.82772
C 8.99619 -0.48963 -1.92463	C -2.34452 0.42783 0.35152	C -0.89835 4.20017 -2.46601
C 8.29287 -1.75759 -2.13355	C -1.59779 -0.13830 1.47924	C 0.13018 4.36134 0.14827
C 9.04420 -2.87258 -1.54825	C -4.44541 -0.19127 1.51010	C 1.00843 4.32091 -0.96483
C 11.11759 0.42784 -1.04502	C -2.29259 -1.28841 2.05739	C 0.49450 4.24015 -2.25298
C 8.26652 0.41314 -1.03189	C -3.69634 -1.31333 2.07603	C 2.47155 4.36989 -0.74777
C 9.00167 0.61827 0.21978	C -1.55165 -2.53084 1.85209	C 2.09396 4.46842 1.70688
C 10.40321 0.65921 0.20635	C -4.39802 -2.58307 1.88746	C 0.63260 4.43516 1.47273
C 11.15098 0.06667 1.31187	C -3.66980 -3.47596 0.98454	H -1.30504 4.13053 -3.46777
C 8.30026 0.04417 1.37320	C -2.26713 -3.44911 0.96715	H 1.18573 4.20551 -3.08667
C 10.45393 -1.05818 1.92786	C -1.55569 -3.64502 -0.29646	C -1.63987 4.43277 2.33444
C 9.05093 -1.08603 1.92765	C -4.40297 -3.69405 -0.26344	C -0.24702 4.46710 2.54768
C 11.19742 -2.28895 1.68389	C -6.55062 -3.15700 -1.37558	H -2.33098 4.45654 3.16862
C 8.34801 -2.35946 1.75430	C -5.85317 -2.01096 -1.96705	H 0.16035 4.51499 3.55045
C 9.07757 -3.23907 0.83720	C -6.59595 -0.76672 -1.75264	N 2.92532 4.40574 0.57704
C 10.48054 -3.22797 0.82849	C -7.99617 -0.78589 -1.74750	N -4.06946 4.21621 -0.49278
C 11.19311 -3.38325 -0.43585	C -8.69987 -2.05879 -1.92328	O 2.57488 4.53258 2.85897
C 8.34353 -3.47382 -0.40935	C -7.94940 -3.18908 -1.36732	O 3.28444 4.38761 -1.69886
C 6.19705 -2.93388 -1.52517	C -5.87936 0.15543 -0.86932	O -3.72121 4.13236 -2.77679
C 6.89385 -1.78128 -2.10594	C -8.72529 0.09442 -0.83173	O -4.43234 4.40509 1.77439
C 6.15033 -0.53671 -1.89965	C -7.99126 0.33195 0.41522	C 4.39064 4.48835 0.79049
C 4.74820 -0.56492 -1.87783	C -6.59247 0.34662 0.39802	C 4.96659 5.90326 0.59902
C 4.04675 -1.83352 -2.07519	C -5.84529 -0.21314 1.52944	C 4.45421 6.96132 1.59171
C 4.79724 -2.95599 -1.50586	C -8.69214 -0.27222 1.55314	N 3.06484 7.40140 1.34083
C 6.86710 0.37799 -1.01044	C -6.54189 -1.36440 2.10945	C 2.92162 8.25571 0.15546
C 4.02125 0.32794 -0.97737	C -7.94155 -1.38724 2.13703	C 2.43462 7.98643 2.53261

C 4.75445 0.55418 0.27046	C -5.79892 -2.61078 1.90960	H 3.46548 9.21795 0.25058
C 6.15426 0.58427 0.25494	C -8.64558 -2.65551 1.93176	H 3.29539 7.74217 -0.73421
C 6.90149 0.01180 1.38142	C -7.91591 -3.55858 1.03806	H 1.86224 8.47950 -0.00635
C 4.05401 -0.03563 1.41695	C -6.51659 -3.52406 1.01690	H 2.93016 8.91701 2.87607
C 6.20491 -1.13477 1.96895	C -5.80374 -3.72314 -0.24806	H 2.45648 7.25693 3.34694
C 4.80332 -1.16072 1.97866	C -8.65071 -3.76076 -0.21366	H 1.38886 8.22488 2.31155
C 6.94830 -2.37928 1.75941	C -10.80019 -3.20954 -1.30584	H 4.57300 4.13359 1.80534
C 4.10209 -2.43034 1.79106	C -10.10245 -2.08580 -1.92364	H 4.85493 3.80561 0.07615
C 4.83065 -3.32186 0.88755	C -10.84540 -0.85434 -1.67939	H 6.05555 5.82054 0.72650
C 6.23129 -3.30149 0.87459	C -12.27252 -0.86741 -1.68676	H 4.80481 6.22154 -0.43644
C 6.94402 -3.48884 -0.39201	C -12.95208 -2.12580 -1.82328	H 4.48321 6.53891 2.60161
C 4.09747 -3.54360 -0.36067	C -12.22574 -3.25352 -1.30848	H 5.14553 7.83042 1.58335
C 1.94912 -3.00960 -1.47441	C -10.12831 0.08379 -0.82330	C -5.53669 4.20659 -0.70811
C 2.64486 -1.85906 -2.05640	C -12.97697 -0.02678 -0.75907	C -6.18346 5.60239 -0.65680
C 1.90410 -0.61824 -1.84135	C -12.26720 0.24001 0.46114	C -5.72201 6.58000 -1.75184
C 0.49790 -0.64403 -1.82461	C -10.84107 0.23896 0.44101	N -4.35772 7.11244 -1.54861
C -0.20231 -1.91060 -2.02287	C -10.09432 -0.28570 1.58043	C -4.26259 8.08992 -0.45745
C 0.54716 -3.03489 -1.45811	C -12.94462 -0.38341 1.56478	C -3.75099 7.60147 -2.79457
C 2.61805 0.30116 -0.96036	C -10.79204 -1.44363 2.12976	H -4.85518 9.00803 -0.64934
C -0.22803 0.24996 -0.92784	C -12.21807 -1.46438 2.17237	H -4.61194 7.65168 0.48115
C 0.50479 0.48014 0.31978	C -10.04818 -2.68749 1.96237	H -3.21670 8.38355 -0.32178
C 1.90575 0.50610 0.30405	C -12.89936 -2.70601 1.93313	H -4.29043 8.46514 -3.23347
C 2.65272 -0.06190 1.43146	C -12.19301 -3.61976 1.07934	H -3.73146 6.79096 -3.52833
C -0.19549 -0.11310 1.46332	C -10.76712 -3.57131 1.05118	H -2.71980 7.91410 -2.59906
C 1.95800 -1.21185 2.00845	C -10.05295 -3.80099 -0.20018	H -7.26675 5.45304 -0.77221
C 0.55274 -1.23724 2.02372	C -12.90452 -3.78443 -0.15835	H -6.03987 6.03040 0.34104
C 2.69895 -2.45440 1.80406	H -14.02728 -0.34702 1.63218	H -5.72640 6.05724 -2.71403
C -0.14720 -2.50520 1.83514	H -13.98067 -2.75847 2.01177	H -6.45645 7.40949 -1.82977
H -5.96703 3.57529 0.07182	H -5.70053 3.74096 -1.68045	

Table S11. Cartesian coordinate from optimized structure of PCBM.

XYZ coordinates of PCBM		
C -0.06678 3.28437 0.56749	C -3.42989 -2.34699 -1.70743	C 1.11690 0.65268 -2.33679
C 0.64573 2.85215 -0.62873	C -2.56723 -1.93005 -2.72471	C -2.90676 -3.10298 -0.57293
C -0.03632 2.77035 -1.84932	C -1.14557 -2.24894 -2.65102	C 3.37988 -1.01914 0.25021
C -1.45539 3.10160 -1.92071	C -0.63944 -2.96357 -1.55747	C 4.47184 0.03397 0.50928
C -2.13552 3.51314 -0.77133	C -1.54292 -3.39940 -0.49966	C 5.41810 0.24889 -0.68753
C -1.42373 3.61183 0.49962	C -3.62632 -2.67619 0.62371	C 6.56602 1.22154 -0.37616
C 0.44850 2.52413 1.69947	C -4.58345 -1.64945 0.23108	C 6.11597 2.65164 -0.18418
C 1.48473 1.62445 1.21452	C -4.46194 -1.44593 -1.21034	O 4.98272 3.09891 -0.39523
C 1.60938 1.83099 -0.24757	C -4.58752 -0.16089 -1.74783	O 7.15372 3.44137 0.25348
C 1.86721 0.76596 -1.10138	C -3.68764 0.27680 -2.80901	C 6.86182 4.86968 0.45492
C 0.20417 1.63993 -2.72418	C -2.70013 -0.58941 -3.28855	H 6.54140 5.32511 -0.48454
C -2.09049 2.16860 -2.84743	C -0.40509 -1.11341 -3.16380	H 7.80043 5.29875 0.79944

C -3.37611 1.68574 -2.58369	C 0.80466 -0.75205 -2.56031	H 6.07462 4.99143 1.20196
C -4.08435 2.11743 -1.38390	C 1.35557 -1.52453 -1.46528	H 7.30076 1.21885 -1.19315
C -3.47701 3.01309 -0.49806	C 0.63181 -2.59386 -0.95324	H 7.11898 0.91286 0.52027
C -3.59863 2.80961 0.94344	C 0.50953 -2.80109 0.50842	H 4.84120 0.63370 -1.53717
C -2.33202 3.18378 1.55980	C -0.83526 -3.29307 0.77057	H 5.85272 -0.70945 -0.99406
C -1.84102 2.45681 2.64766	C -1.53072 -2.89506 1.91977	H 5.05045 -0.30331 1.38078
C -0.42234 2.12505 2.72140	C -2.95215 -2.57527 1.84362	H 4.01815 0.99147 0.77581
C 1.62116 0.35926 1.77277	C -4.82544 -0.55916 1.07286	C 4.22711 -2.98731 -1.12592
C 0.68347 -0.07200 2.79063	C -4.12186 -0.45107 2.34596	C 4.81136 -4.25640 -1.21404
C -0.30260 0.79210 3.27899	C -3.20675 -1.43845 2.72428	C 5.10078 -4.97972 -0.05222
C -1.64401 0.28854 3.55765	C -1.94156 -1.05871 3.34235	C 4.80345 -4.42758 1.19980
C -2.59755 1.31990 3.16503	C -0.91071 -1.96148 2.83910	C 4.22057 -3.16002 1.28665
C -3.81062 0.95793 2.57103	C 0.37318 -1.47694 2.56556	C 3.92505 -2.42524 0.12513
C -4.32210 1.71912 1.43679	C 1.11492 -1.93074 1.40593	H 3.99680 -2.43652 -2.03182
C -4.95114 0.78217 0.51124	C 2.05361 -0.84113 0.98937	H 5.03585 -4.67830 -2.18852
C -4.83484 0.97692 -0.86779	C 2.19258 -0.61539 -0.61850	H 5.55012 -5.96520 -0.12077
C -1.06164 1.26314 -3.34615	C -1.35976 -0.08381 -3.56220	H 5.02092 -4.98411 2.10590
H 3.98569 -2.73894 2.25961		

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