Electronic Supplementary Information

Benzene-Fused Porphyrin(2.1.2.1) Array: Synthesis, Structure, and Electrocatalytic Hydrogen Evolution

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1, Instrument and Materials. Absorption spectra were measured with a JASCO UV/VIS/NIR Spectrophotometer V-670. The UV absorption spectrum in film state was measured at normal incidence at room temperature, **BPD** was dissolved in CH_2Cl_2 to prepare a solution with a concentration of 2.528×10^{-5} mol/ml, which was evenly coated on the quartz substrate to obtain a thin film. A blank quartz identical substrate to the one used for the thin film deposition was used as a reference for the absorption scan. APCI-FT-MS mass spectrum was recorded on a Ther-moFisher Scientific spectrometer. The cyclic voltammetry was conducted in a solution of 0.1 M TBAP in dry-CH_2Cl_2 (distilled from CaH under reduced pressure) with a scan rate of 0.1 V s^{-1} in an N_2-filled cell. A glassy carbon electrode and a platinum wire were used as a working and a counter electrode, respectively. A saturated Calomel electrode (SCE) was used as reference electrodes. Other organic solvents and chemicals were reagent grade quality, obtained commercially and used without further purification. X-ray crystallographic data for **BPD** (CCDC: 2323090) was recorded on a BRUKER D8 VENTURE TXS PHOTON 100 diffractometer. The crystal was kept at 202.20 K during data collection. Using Olex2[1], the structure was solved with the SHELXT[2] structure solution program using Intrinsic Phasing and refined with the SHELXL[3] refinement package using Least Squares minimisation. Electron paramagnetic resonance (EPR) were measured by BRUKE EMXplus. Experiment parameters: FrequencyMon 9.292044 GHz, ModAmp 4.000 G, ModFreq 100.00 kHz. All density functional theory calculations were achieved with the Gaussian 09 program package.[4] The singlet and triplet multiplicity geometries of **BPD** were optimized using density functional theory (DFT) at the level of UB3LYP/6-31G(d, p).

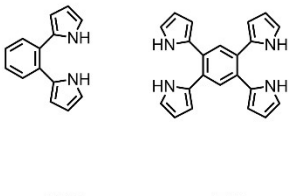
2, Electrochemical Study. The linear sweep voltammograms (LSVs) were acquired in 0.50 M H_2SO_4 using a three-compartment cell with a glassy carbon working electrode, a graphite rod auxiliary electrode, and a Ag/AgCl (saturated with KCl) reference electrode. The preparation of catalyst-coated glassy carbon electrode is described as follows. To 1.0 mL freshly distilled acetonitrile, were added 1.0 mg CNTs, 1.0 mg **BP** or **BPD**, and 25 μL Nafion (5.0 wt%, DuPont). The resulted mixture was sonicated using an ultrasonic cleaner for 30 min to get an ink. Then, 4 μL of the suspension was dropped onto the surface of a freshly polished glassy carbon electrode. After drying at room temperature, the prepared glassy carbon electrodes were used for electrochemical studies. The aqueous 0.50 M H_2SO_4 solution was bubbled with N_2 for 30 min before analysis. The electrolysis of **BP**/CNT and **BPD** /CNT was performed with a three electrode H-type cell containing a Nafion membrane (Nafion®117, DuPont, Inc.) to separate the carbon paper (0.5 cm^2, loading with catalysts) working electrode and the other two electrodes.

3, Synthesis

A solution of **DPB** (208 mg, 1.0 mmol), **TPB** (169 mg, 0.5 mmol), and pentafluorobenzaldehyde (390 mg, 2 mmol) in CH_2Cl_2 (120 ml) was bubbled with N_2 for 5 min, then BF_3•OEt_2 (70 mol%, 50 mg, 0.35 mmol) was added into reaction mixture. The reaction mixture was stirred at room temperature for 3 hours under a N_2 atmosphere in the dark. The DDQ (224 mg, 1.0 mmol) was added to the reaction mixture, which was stirred for 1 hour. Then saturated solution of $Cu(OAc)_2$•$1H_2O$ in MeOH (10 mL) was added to the reaction mixture and it was stirred for 1 h. After removal of the solvent, the residue was purified by alumina column (CH_2Cl_2) and silica gel column chromatographies (*n*-hexane: CH_2Cl_2 = 5 :1). The brown-red fraction was collected to give **BPD** as red solid in 7 % (55 mg, 0.035 mmol).

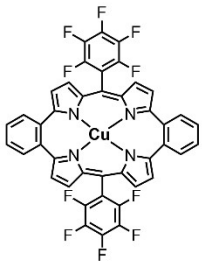
BPD: HR-APCI-MS: *m/z* = 1581.0567 (calcd. for $C_{78}H_{26}Cu_2F_{20}N_8$+H = 1581.0626 $[M+H]^+$). UV-Vis-NIR (in CH_2Cl_2) λ [nm] (ε [$M^{-1}cm^{-1}$]): 534 (144000) nm.

4. Abbreviations

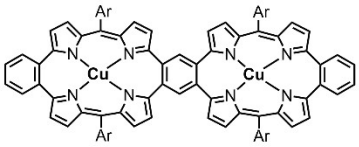


DPB

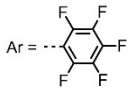
TPB

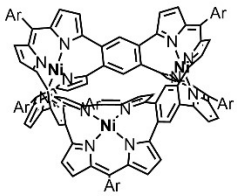


BP

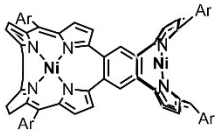


BPD



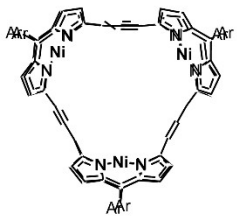


front view

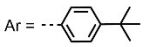


side front

BPN



top view



5. Supporting Figures and Tables

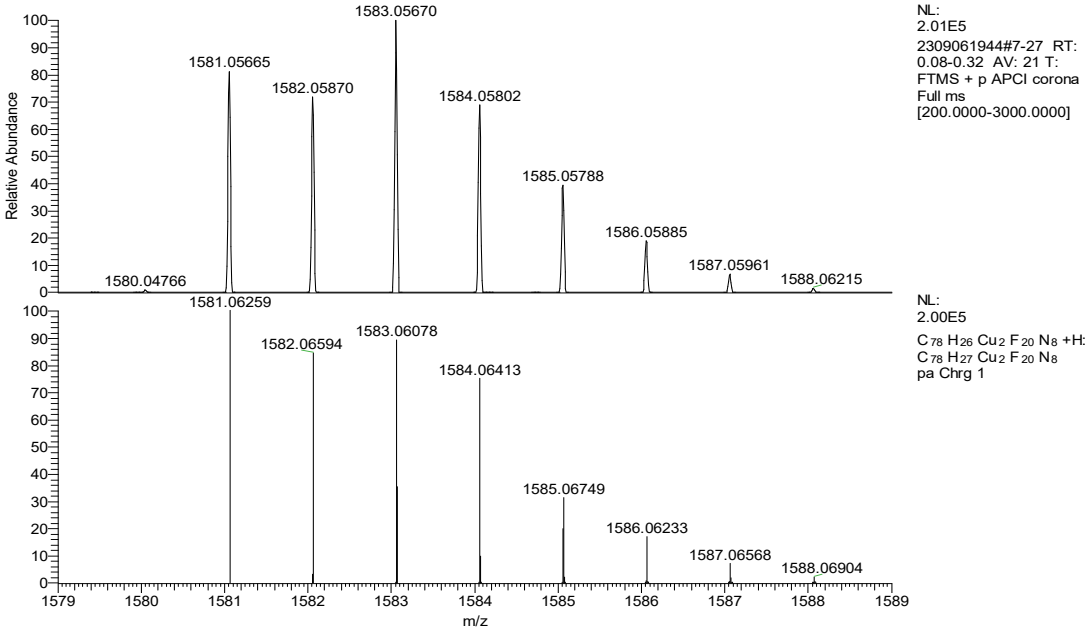


Figure S1. HR-APCI-MS spectrum of **BPD**.

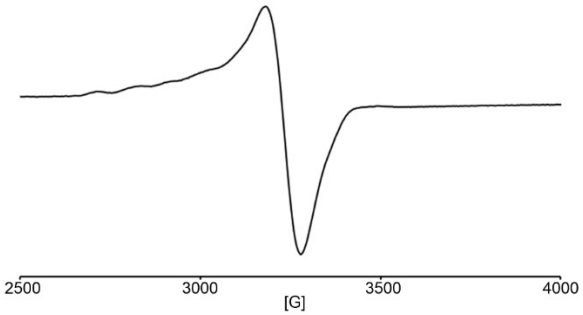


Figure S2. EPR spectrum of **BPD** in CH_2Cl_2 at 110K.

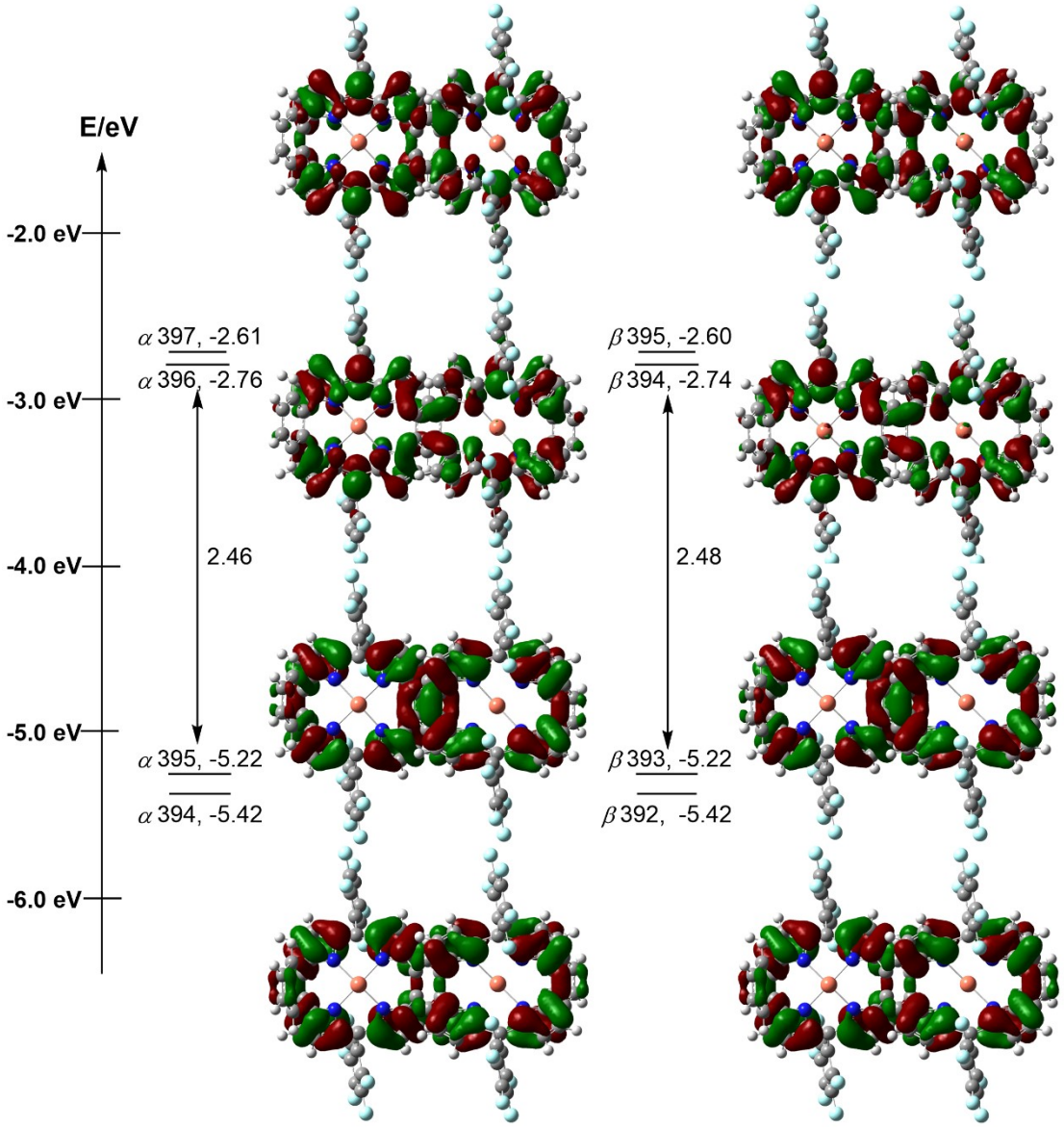


Figure S3. Frontier molecular orbitals and energy diagrams of **BPD** at triplet state, calculated at the UB3LYP/6-31G(d, p) level of theory.

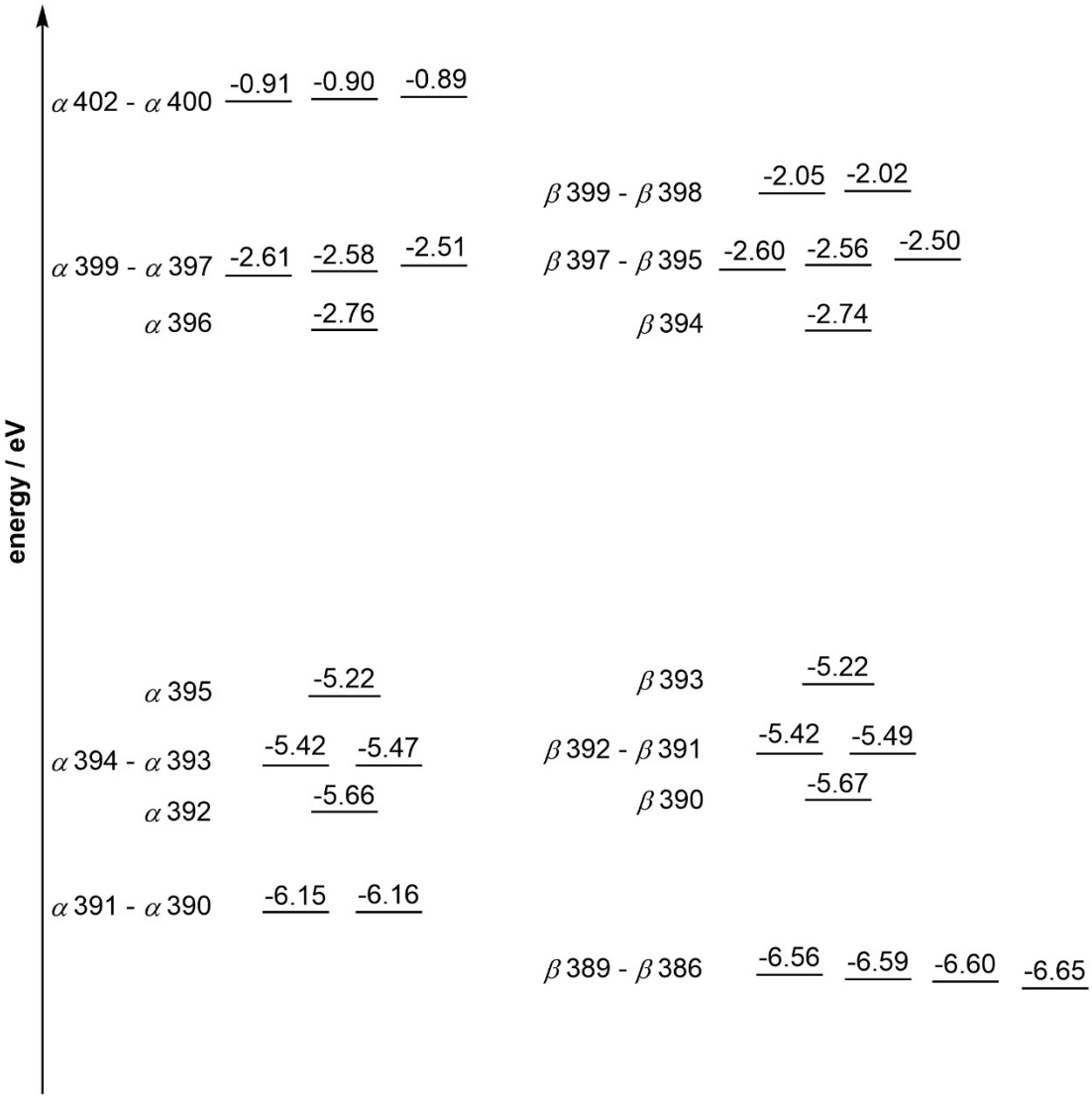


Figure S4. Energy diagrams of **BPD** at triplet state, calculated at the UB3LYP/6-31G(d, p) level of theory.

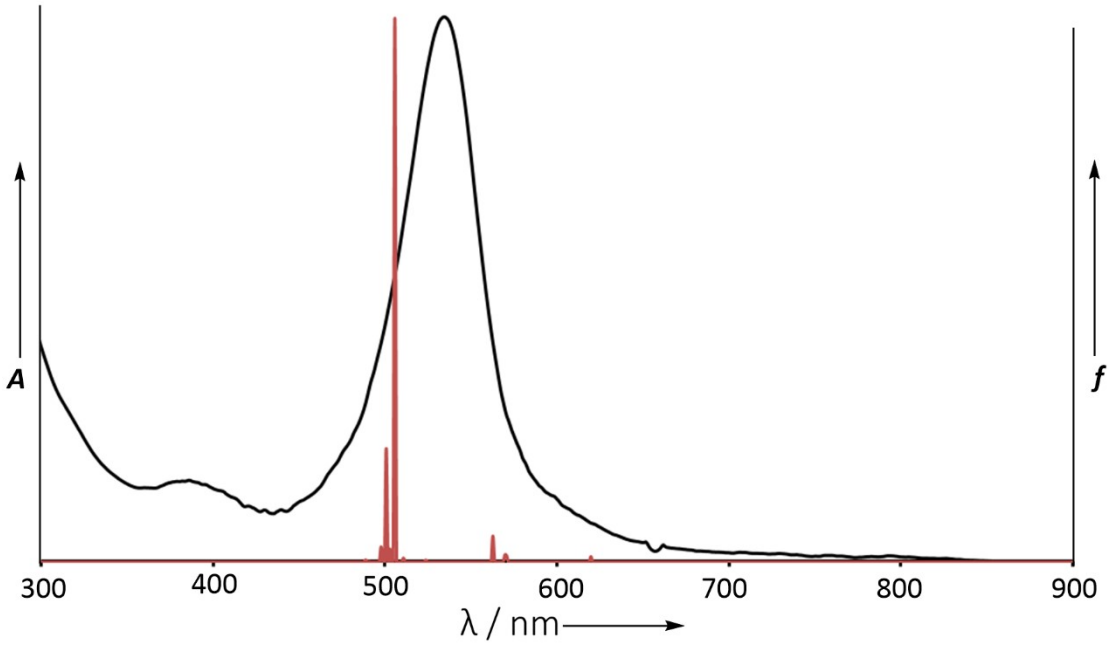


Figure S5. The UV-Vis absorption spectrum (black line, left axis) and oscillator strengths (red bar, right axis), which is calculated by UB3LYP/6-31G(d,p) level of theory of **BPD** at triplet state.

Table S1. Major composition, vertical excitation energies (*E*, eV/nm) and oscillator strengths (*f*) for the lowest optically allowed excited states of **BPD** at triplet state, calculated at the UB3LYP/6-31G(d,p) level of theory.

State	Major Composition	**Exci.** (eV/nm)	*f*
1	395A -> 397A (0.42919) 393B -> 395B (-0.42645) 393A -> 396A (0.37536)	1.4707/853.05	0.0002
2	395A -> 396A (0.69562) 393B -> 394B (0.66463)	2.0012/619.56	0.0044
3	391B -> 394B (0.60898) 393B -> 395B (0.71336)	2.2007/563.40	0.0213
4	393A -> 396A (0.45848) 394A -> 399A (0.49493) 395A -> 397A (0.50807)	2.4513/505.78	0.4441

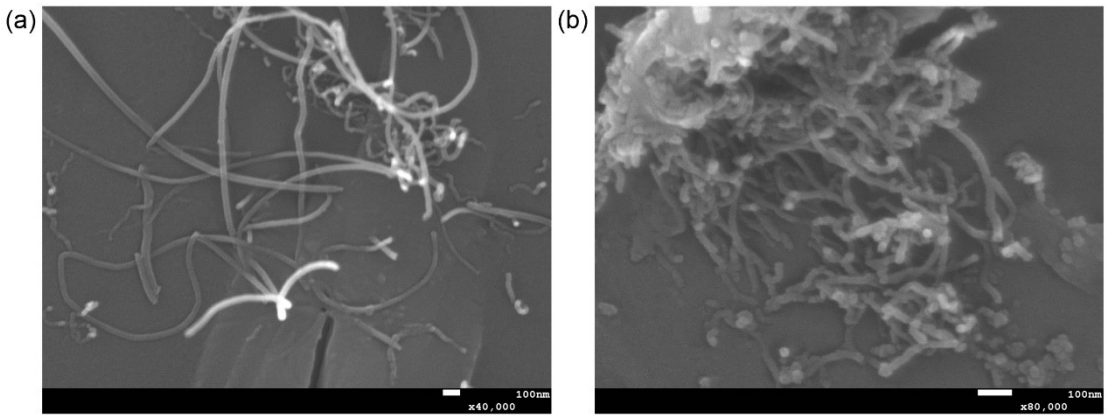


Figure S6. SEM images of (a) **BP/CNT** and (b) **BPD/CNT**.

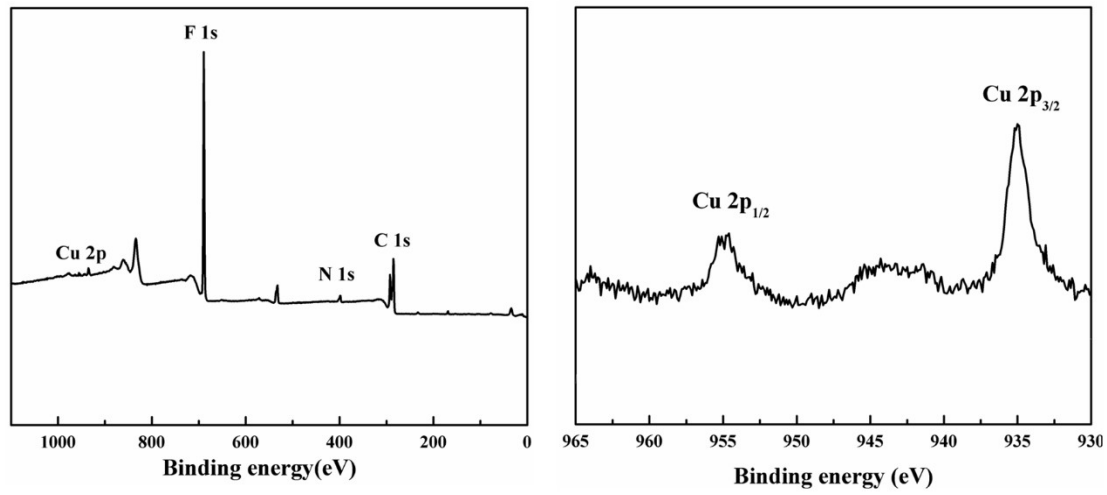


Figure S7 XPS scan spectrum of **BP/CNT** and the corresponding Cu 2p binding energy region.

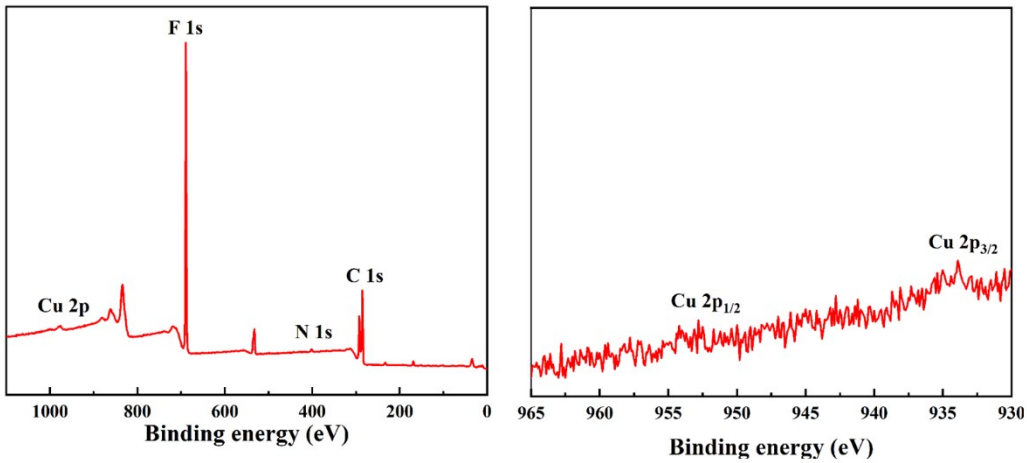


Figure S8 XPS scan spectrum of **BPD/CNT** and the corresponding Cu 2p binding energy region.

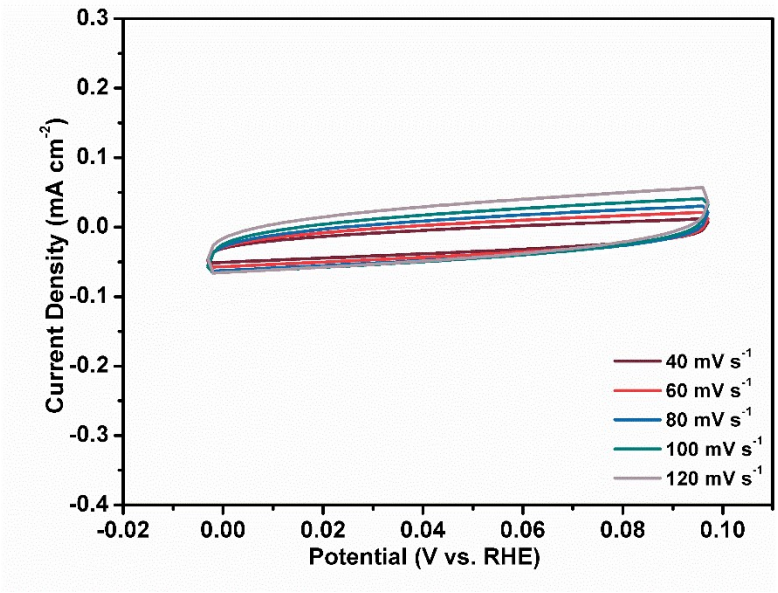


Figure S9. CVs at different scan rates of **BP/CNT**.

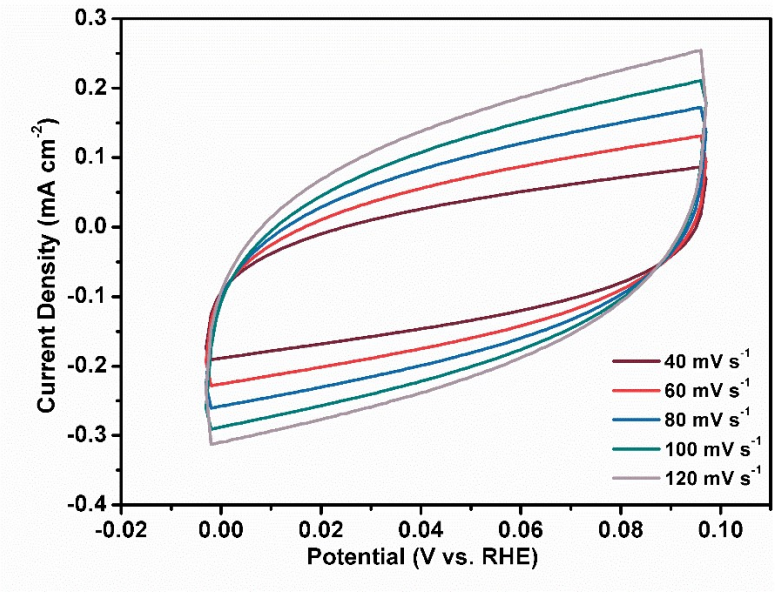


Figure S10. CVs at different scan rates of **BPD/CNT**.

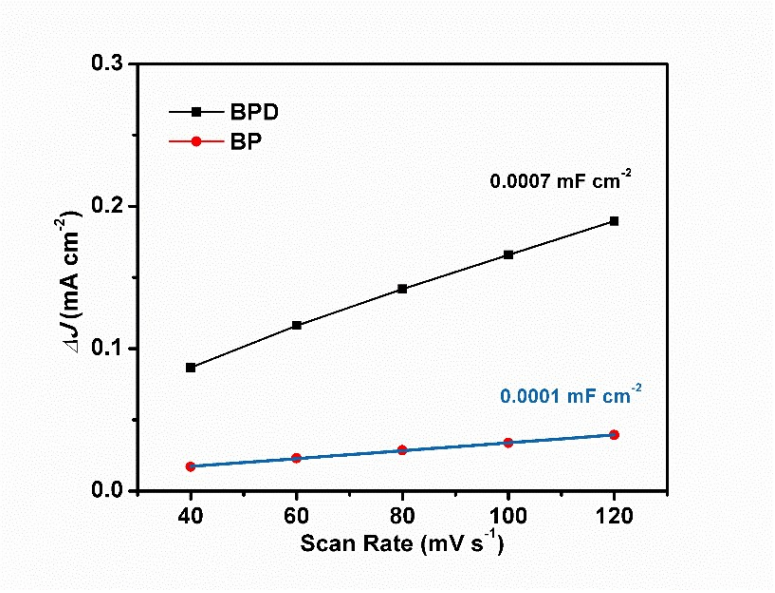


Figure S11. Linear fitting of the current densities vs scan rates for **BP/CNT** and **BPD/CNT**.

6, Crystal Data

Table S2. Crystal data of **BPD**.

Empirical formula	$C_{91}H_{60}Cl_2F_{20}N_8O_2Rh_2$
Formula weight	1954.19
Temperature/K	202.20
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.46(2)
b/Å	22.68(3)
c/Å	14.222(19)
α/°	90
β/°	95.69(4)
γ/°	90
Volume/Å^3	5605(12)
Z	2
ρ_{calc}g/cm^3	1.158
μ/mm^{-1}	0.416
F(000)	1964.0
Crystal size/mm^3	0.13 × 0.12 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.958 to 41.632
Index ranges	$-16 \le h \le 17$, $-22 \le k \le 20$, $-14 \le l \le 14$
Reflections collected	15093
Independent reflections	5841 [R_{int} = 0.0571, R_{sigma} = 0.0730]
Data/restraints/parameters	5841/1624/648
Goodness-of-fit on F^2	1.163
Final *R* indexes [$I>=2\sigma(I)$]	R_1 = 0.1420, wR_2 = 0.3332
Final *R* indexes [all data]	R_1 = 0.1711, wR_2 = 0.3514
Largest diff. peak/hole / e Å^{-3}	0.69/-0.87

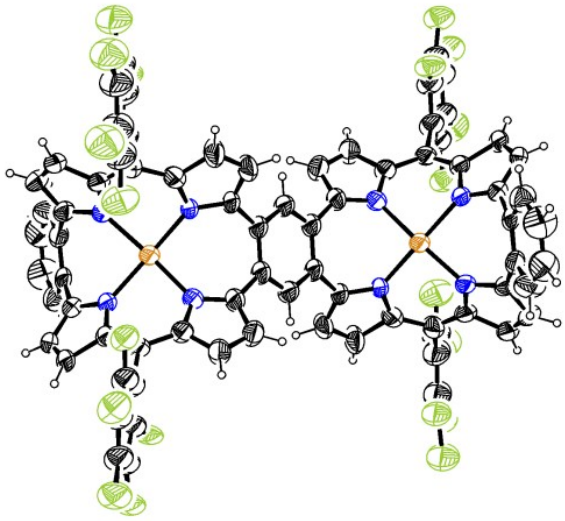


Figure S12 Crystal structure of **BPD**, solvents are omitted for clarity. The thermal ellipsoids represent for 30% probability.

7. Cartesian Coordinates

BPD
Charge = 0
Spin = Triplet
Total energy: E = -8703.31765364 a.u.

C	-6.04772100	1.50234500	3.22121200
C	-6.01278900	-1.50241900	3.25326800
N	-5.48643200	-1.40384400	2.01922400
C	-6.09903800	-2.38557500	1.24376400
C	-7.07410300	-3.06679300	2.03440700
C	-6.99501500	-2.53528800	3.30238800
C	-7.07344600	2.49386900	3.23973300
C	-7.15211000	3.00576500	1.96434300
C	-6.13233200	2.35975700	1.20013200
N	-5.49559000	1.41016500	1.99913800
C	-5.61940400	0.72297600	4.39419800
C	-5.60093400	-0.68912700	4.40847200
N	-3.59269300	1.39688300	-0.00927500
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C	-2.40355600	-2.52455300	-1.59782200
C	-3.67632500	-3.05028000	-1.60395700
C	-4.39775500	-2.38869600	-0.56413100
N	-3.58098100	-1.41786600	0.01308900
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C	-2.38584100	1.50911900	-0.59552000
C	-5.61842900	-2.79557400	-0.00763200
C	-5.64101100	2.76507900	-0.04713300
C	-4.96691900	0.74783800	6.74287200
C	-4.94775500	-0.64782600	6.75698300
C	-5.27227900	-1.35361500	5.60219000
C	-5.30992800	1.42070300	5.57375700
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C	-7.55503000	-3.46441400	-1.45832400
C	-8.32250800	-4.40172800	-2.14576600
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C	-7.15628600	6.07686800	-1.19843000
C	-7.89609300	5.66624200	-2.30485200
C	-7.90601600	4.32333600	-2.67454600
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Cu	-4.39589100	-0.00212800	1.14083000
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F	-7.14239700	7.36706500	-0.84581600
F	-8.59604900	6.55843000	-3.00927100
F	-8.61760600	3.92862300	-3.73549200
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F	-9.40683600	-4.02210400	-2.82979800
F	-8.68222000	-6.65183100	-2.77144400
F	-6.47117900	-7.42964300	-1.37347800
F	-4.99380500	-5.59715000	-0.04426700
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C	5.30998200	-1.42076000	-5.57378300
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C	7.07357000	-2.49381200	-3.23976100
C	7.15224900	-3.00570600	-1.96437400
C	6.13240800	-2.35977400	-1.20017100
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H	4.71811700	-1.30999300	-7.63792500
H	5.33449100	-2.50601200	-5.55823800
H	7.70494700	3.87664600	-1.69724800
H	7.56709400	2.81098100	-4.17714900
H	7.67325700	-2.75504000	-4.10032300
H	7.81958100	-3.77569700	-1.60536500

BPD
Charge = 0

Spin = Singlet
Total energy: E = -8703. 24365606 a.u.

C	-5.98650200	1.45663500	3.29376500
C	-6.03501100	-1.54768500	3.22262800
N	-5.48654700	-1.44388200	2.00107900
C	-6.13539000	-2.36975200	1.18660900
C	-7.16030700	-3.01795300	1.94390000
C	-7.07119800	-2.53000200	3.22779100
C	-6.95837600	2.49921000	3.36300600
C	-7.05393600	3.03609400	2.09836200
C	-6.09631600	2.35079000	1.28908000
N	-5.48246800	1.36221000	2.05088000
C	-5.57258600	0.62615200	4.43564900
C	-5.59880800	-0.78570300	4.40391500
N	-3.57497400	1.41061000	0.05257700
C	-4.41065000	2.36124000	-0.53199200
C	-3.70963200	3.00595900	-1.59681100
C	-2.43385200	2.48738600	-1.60220300
C	-2.40808300	-2.52041300	-1.60704200
C	-3.68922300	-3.02697400	-1.63324800
C	-4.41608100	-2.35723700	-0.60267000
N	-3.59081700	-1.40875800	-0.00668600
C	-2.38711800	-1.51098800	-0.60052000
C	-2.39126200	1.49279800	-0.58099800
C	-5.65078800	-2.75731200	-0.06847600
C	-5.62653200	2.76650900	0.03519400
C	-4.90870400	0.55125200	6.78041900
C	-4.93638000	-0.84390400	6.74907800
C	-5.28856600	-1.50002400	5.57305000
C	-5.23439500	1.27345100	5.63603800
C	-6.44353800	-3.75294600	-0.85458400
C	-6.43245000	3.79828000	-0.68825500
C	-7.18197600	-3.34444000	-1.96898200
C	-7.92531500	-4.24493900	-2.72832700
C	-7.93437600	-5.59335700	-2.37924000
C	-7.20471800	-6.03047500	-1.27624200
C	-6.46867200	-5.11189200	-0.53113400
C	-6.07724000	5.14947300	-0.70180000
C	-6.84004000	6.10248100	-1.37312800
C	-7.99320900	5.70873200	-2.04790800
C	-8.37443000	4.36901100	-2.04896600
C	-7.59680100	3.43363300	-1.37041700
Cu	-4.38809700	-0.02216200	1.15279300
F	-4.97993600	5.56190600	-0.05418100
F	-6.47647900	7.38966800	-1.36707700
F	-8.73166900	6.61402400	-2.69381700
F	-9.48028400	3.99060600	-2.69832600
F	-7.98515700	2.15263400	-1.39294100
F	-8.62725100	-3.82482200	-3.78591100
F	-8.64278500	-6.46554200	-3.10001800

F	-7.20900000	-7.32599600	-0.94352000
F	-5.77067500	-5.56582000	0.51800000
F	-7.19569400	-2.05404400	-2.32535200
C	-1.20404400	0.69620100	-0.24040800
C	-1.20386900	-0.71622100	-0.24364200
C	5.62668200	2.76652400	-0.03510000
C	5.65068500	-2.75772300	0.06830300
C	0.00008400	1.36923000	0.00014300
C	1.20417900	0.69602400	0.24052000
C	1.20382700	-0.71640800	0.24339900
C	-0.00006600	-1.38908300	-0.00019400
C	2.39140500	1.49259500	0.58114200
C	2.38693200	-1.51146300	0.60011400
N	3.59062900	-1.40935200	0.00629800
C	4.41586000	-2.35782300	0.60235000
C	3.68887900	-3.02761200	1.63281000
C	2.40777500	-2.52096700	1.60658100
C	2.43390600	2.48733700	1.60218100
C	3.70964200	3.00603700	1.59672900
C	4.41074200	2.36125800	0.53202100
N	3.57515500	1.41047700	-0.05243600
C	5.59897300	-0.78554500	-4.40383200
C	5.57290500	0.62631400	-4.43550700
C	5.23477100	1.27370300	-5.63587000
C	4.90901700	0.55159400	-6.78028300
C	4.93657300	-0.84356900	-6.74901100
C	5.28868100	-1.49977500	-5.57301200
N	5.48316900	1.36197200	-2.05063600
C	6.09670800	2.35074500	-1.28887500
C	7.05406300	3.03638100	-2.09823800
C	6.95846400	2.49957600	-3.36289900
C	7.07117000	-2.53002600	-3.22786800
C	7.16026800	-3.01811500	-1.94402900
C	6.13537600	-2.36993000	-1.18668700
N	5.48664300	-1.44387600	-2.00100300
C	6.03507700	-1.54763700	-3.22259500
C	5.98687700	1.45669800	-3.29360000
C	6.44340000	-3.75330600	0.85447500
C	6.43245800	3.79848000	0.68829800
C	6.07693500	5.14960200	0.70193200
C	6.83966500	6.10276100	1.37310400
C	7.99306200	5.70925100	2.04765900
C	8.37457900	4.36962700	2.04863000
C	7.59701400	3.43408400	1.37021300
C	7.18092100	-3.34485900	1.96952600
C	7.93429200	-5.59352600	2.37937400
C	7.20555100	-6.03059500	1.27575500
C	6.46944100	-5.11212800	0.53056700
Cu	4.38812300	-0.02211600	-1.15238300
F	4.97939700	5.56177600	0.05454700

F	6.47585800	7.38988100	1.36713100
F	8.73143900	6.61471700	2.69342400
F	9.48064500	3.99144300	2.69775700
F	7.98568200	2.15317500	1.39264200
F	7.19376400	-2.05459500	2.32640500
F	8.64272200	-6.46560700	3.10025200
F	5.77223200	-5.56610200	-0.51908000
F	7.21070500	-7.32598700	0.94253800
C	7.92428400	-4.24524500	2.72897200
F	8.62534500	-3.82515200	3.78714700
H	-7.83568300	-3.77619300	1.57473800
H	-7.67268300	-2.79770400	4.08525000
H	-7.51752900	2.77309400	4.24677700
H	-7.68003400	3.85580900	1.77588500
H	-4.10646600	3.77891200	-2.23908100
H	-1.61306300	2.74488700	-2.25685800
H	-1.57059600	-2.79432700	-2.23325200
H	-4.07276800	-3.81560000	-2.26486100
H	-4.63738300	1.07500100	7.69199700
H	-4.68719000	-1.41858500	7.63593900
H	-5.31947800	-2.58484200	5.54396500
H	-5.22222300	2.35876300	5.65646300
H	0.00014000	2.45451200	0.00025000
H	-0.00011500	-2.47432300	-0.00031200
H	4.07229500	-3.81638600	2.26432000
H	1.57023200	-2.79488700	2.23271500
H	1.61310600	2.74482500	2.25682700
H	4.10639600	3.77911400	2.23889800
H	5.22268800	2.35901600	-5.65623700
H	4.63773700	1.07541000	-7.69183400
H	4.68735000	-1.41818200	-7.63590700
H	5.31948600	-2.58459600	-5.54397300
H	7.68000400	3.85622500	-1.77578700
H	7.51744300	2.77365200	-4.24671900
H	7.67264700	-2.79767300	-4.08535000
H	7.83559400	-3.77645700	-1.57499400

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