

Supporting Information:

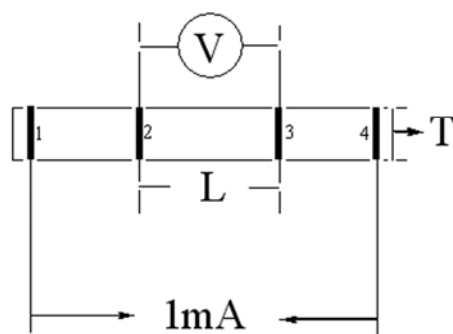
Novel Electroactive Proton-Doped Conducting Poly(aromatic ethers) with Good Fluorescence Properties via Electropolymerization

Baoyang Lu,[†] Jun Yan,[‡] Jingkun Xu,^{*,†} Shuyun Zhou,^{*,‡} and Xiujie Hu[‡]

[†]*Jiangxi Key Laboratory of Organic Chemistry, Jiangxi Science and Technology
Normal University, Nanchang 330013, China, and* [‡]*Key Laboratory of Photochemical
Conversion and Optoelectronic Materials, Technical Institute of Physics and Chemistry,
Chinese Academy of Sciences, Beijing 100190, China*

*: Corresponding author. Tel: 86–791–8537029, Fax: 86–791–3823357, Email:

xujingkun@tsinghua.org.cn and zhou_shuyun@mail.ipc.ac.cn.



Scheme S1 The arrangement of four probes in the electrical conductivity measurements of the polymers. The applied current (I) was 1 mA by the use of 220 Programmable Current Source between 1 and 4, and the voltage (V) between 2 and 3 is measured by a Keithley 2700 multimeter. L denotes to the distance between 2 and 3, while T and ϕ denote the width and thickness of the sample, respectively. Copper wires were used as the probes, and pressed by high purity silver paint onto the polymer thin films/pressed pellets to ensure good contact.

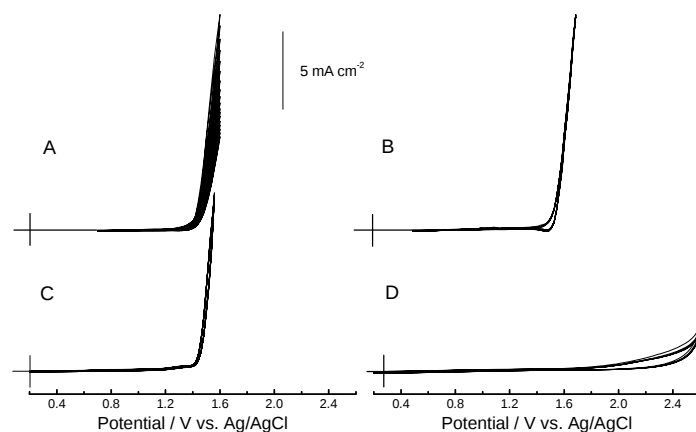


Figure S1 Cyclic voltammograms of DNE (A), DPOB (B), DPS (C), and DPSO (D) in acetonitrile solution containing $0.1 \text{ mol L}^{-1} \text{ Bu}_4\text{NBF}_4$. Monomer concentration: 0.02 mol L^{-1} . Potential scan rate: 100 mV s^{-1} .

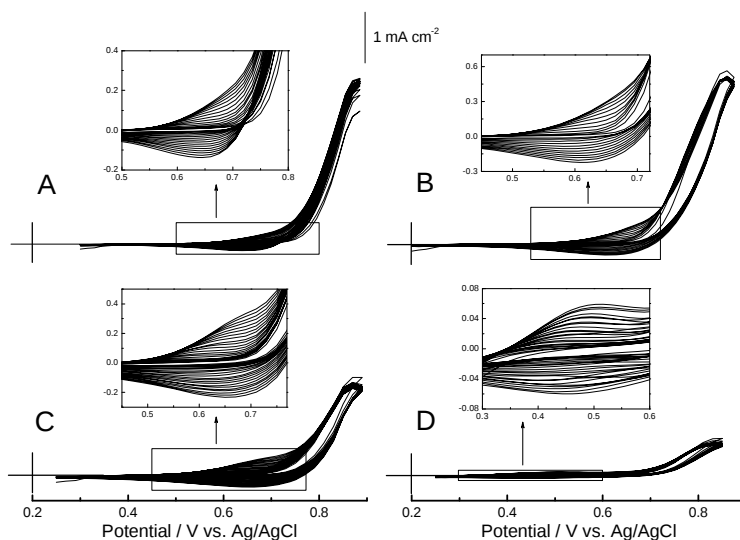


Figure S2 Cyclic voltammograms of DNE in the mixed electrolytes of BFEE and SA: 5% (A), 10% (B), 15% (C), 20% (D) (ratio of SA, by volume). Monomer concentration:

0.02 mol L⁻¹. Potential scan rate: 100 mV s⁻¹.

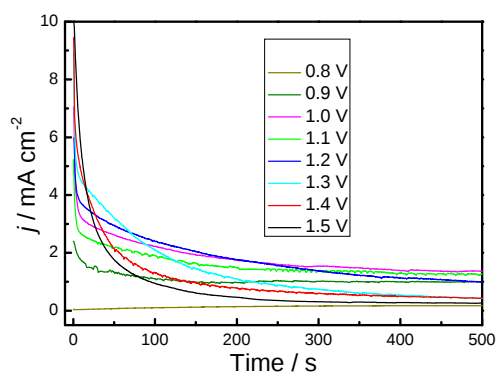


Figure S3 Chronamperograms of 0.02 mol L⁻¹ DNE in BFEE on a Pt electrode at the applied potentials indicated.

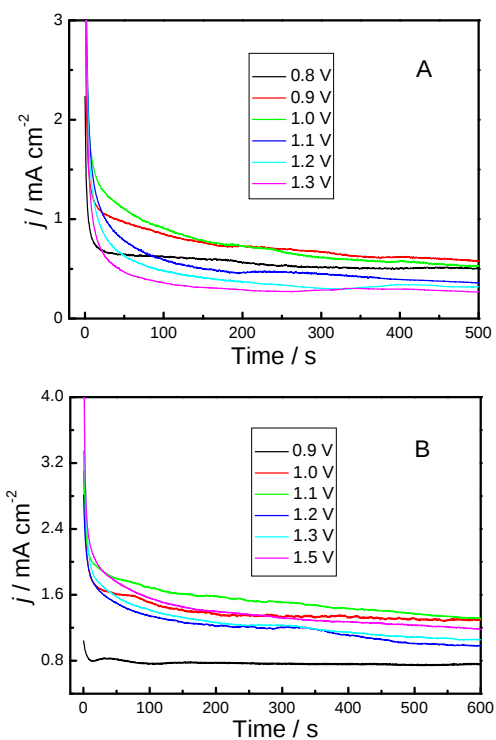
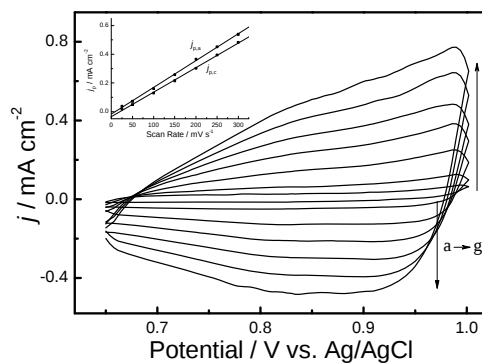


Figure S4 Chronamperograms of 0.02 mol L⁻¹ DNE in BFEE containing 10% SA (A) and 0.02 mol L⁻¹ DPOB in BFEE (B) on Pt electrodes at the applied potentials indicated.



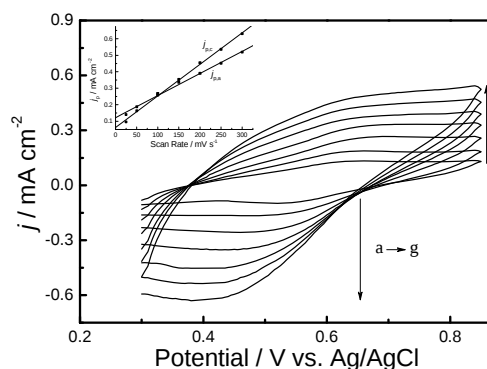
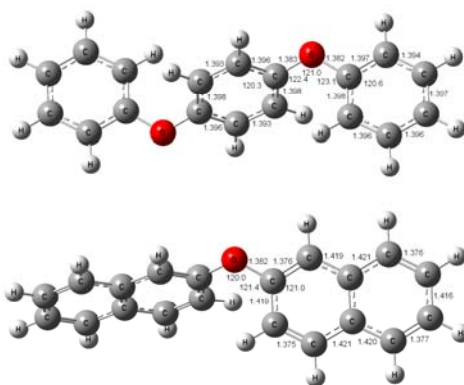
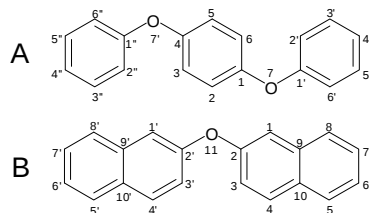


Figure S5 Cyclic voltammograms of PDNE films electrochemically synthesized in BFEE on the Pt electrode in monomer-free BFEE (A) and in concentrated SA (B) at potential scan rates of 25, 50, 100, 150, 200, 250, and 300 mV s^{-1} . Inset: plots of redox peak current densities vs. potential scan rates. j_p is the peak current density, and $j_{p,a}$ and $j_{p,c}$ denote the anodic and cathodic peak current densities, respectively.



Scheme S2 Calculated (B3LYP/6-31G(d)) optimized geometries DPOB and DNE.



Scheme S3 The numbering of the atoms in DPOB (A) and DNE (B).

Table S1 Main atomic electron density populations for DPOB and DNE.

DPOB		DNE	
Atom	Electric charge	Atom	Electric charge
C ₍₁₎	0.316676	C ₍₁₎	-0.174824
C ₍₂₎	-0.123065	C ₍₂₎	0.314465
C ₍₃₎	-0.110725	C ₍₃₎	-0.106264
C ₍₄₎	0.316796	C ₍₄₎	-0.141692
C ₍₅₎	-0.123134	C ₍₅₎	-0.130297
C ₍₆₎	-0.110578	C ₍₆₎	-0.092881
C _(1')	0.316817	C ₍₇₎	-0.092026
C _(2')	-0.114821	C ₍₈₎	-0.128668

C _(3')	-0.092087	C ₍₉₎	0.097417
C _(4')	-0.085832	C ₍₁₀₎	0.108654
C _(5')	-0.095175	C _(1')	-0.174821
C _(6')	-0.110528	C _(2')	0.314452
C _(1'')	0.316721	C _(3')	-0.106250
C _(2'')	-0.110364	C _(4')	-0.141688
C _(3'')	-0.095164	C _(5')	-0.130298
C _(4'')	-0.085809	C _(6')	-0.092879
C _(5'')	-0.092102	C _(7')	-0.092027
C _(6'')	-0.114800	C _(8')	-0.128666
O ₍₇₎	-0.576057	C _(9')	0.097414
O _(7')	-0.576046	C _(10')	0.108654
		O ₍₁₁₎	-0.575529

Table S2 Main composition and proportion of the Frontier Orbitals in DPOB(%).

Atom	HOMO-1	HOMO	LUMO	LUMO+1
C ₍₁₎	0.954859	9.203599	1.108743	16.43025
C ₍₂₎	0.979301	3.643109	14.21746	6.543448
C ₍₃₎	1.416659	5.412335	19.19455	2.033422
C ₍₄₎	0.94434	9.196119	1.113528	16.43375
C ₍₅₎	1.006624	3.639787	14.21939	6.544608
C ₍₆₎	1.406482	5.402528	19.20038	2.02844
C _(1')	9.251286	3.862156	0.520134	8.471821
C _(2')	4.729414	4.157553	3.96897	2.05019
C _(3')	2.388591	0.367581	3.978244	1.791804
C _(4')	11.56108	4.755223	0.081374	6.857786
C _(5')	1.669887	0.725174	3.681774	1.374033
C _(6')	5.45726	2.794167	2.844858	2.335705
C _(1'')	9.194723	3.837032	0.526965	8.573179
C _(2'')	4.722682	4.141651	4.014616	2.032923
C _(3'')	2.362348	0.362156	3.999404	1.865351
C _(4'')	11.49592	4.721448	0.081919	6.969831
C _(5'')	1.667342	0.725015	3.721896	1.360764
C _(6'')	5.423444	2.776745	2.859092	2.41453
O ₍₇₎	11.54496	14.79013	0.043096	1.569187
O _(7')	11.54038	14.76173	0.043093	1.576099

Table S3 Main composition and proportion of the Frontier Orbitals in DNE(%).

Atom	HOMO-1	HOMO	LUMO	LUMO+1
C ₍₁₎	8.372049	10.88409	8.928775	6.168145
C ₍₂₎	5.452996	6.457567	2.745162	2.719687

C ₍₃₎	2.959043	1.068008	5.031058	6.45477
C ₍₄₎	7.231731	4.543292	10.82713	7.86909
C ₍₅₎	8.10783	3.905745	7.52315	9.248912
C ₍₆₎	4.571226	6.104157	2.913108	2.468394
C ₍₇₎	2.926443	0.556593	4.117264	5.191962
C ₍₈₎	8.694236	6.376628	7.095201	8.561878
C ₍₉₎	0.138618	0.768556	0.326556	0.089857
C ₍₁₀₎	0.066424	1.827473	0.155747	0.436272
C _(1')	8.382359	10.87366	8.932678	6.164693
C _(2')	5.458038	6.451884	2.746675	2.719476
C _(3')	2.960429	1.068873	5.03396	6.451116
C _(4')	7.239054	4.537082	10.83182	7.863903
C _(5')	8.116578	3.900217	7.527569	9.244767
C _(6')	4.576943	6.098415	2.914188	2.467867
C _(7')	2.92905	0.555452	4.119567	5.189464
C _(8')	8.703207	6.368905	7.098994	8.558523
C _(9')	0.138883	0.768439	0.326782	0.089686
C _(10')	0.06661	1.826356	0.155882	0.435996
O ₍₁₁₎	2.660939	14.77882	0.531106	1.354541

Table S4 Main atomic electron spin densities for DPOB and DNE.

DPOB		DNE	
Atom	Electric spin density	Atom	Electric spin density
C ₍₁₎	0.160239	C ₍₁₎	0.188215
C ₍₂₎	0.044409	C ₍₂₎	0.039629
C ₍₃₎	0.025810	C ₍₃₎	-0.021025
C ₍₄₎	0.160238	C ₍₄₎	0.053434
C ₍₅₎	0.044411	C ₍₅₎	0.017961
C ₍₆₎	0.025809	C ₍₆₎	0.116936
C _(1')	0.010947	C ₍₇₎	-0.057334
C _(2')	0.045979	C ₍₈₎	0.141168
C _(3')	-0.024875	C ₍₉₎	-0.052477
C _(4')	0.072756	C ₍₁₀₎	0.024881
C _(5')	-0.016776	C _(1')	0.188098
C _(6')	0.034418	C _(2')	0.039608
C _(1'')	0.010947	C _(3')	-0.021005
C _(2'')	0.045985	C _(4')	0.053387
C _(3'')	-0.024878	C _(5')	0.017949
C _(4'')	0.072767	C _(6')	0.116882
C _(5'')	-0.016781	C _(7')	-0.057308
C _(6'')	0.034426	C _(8')	0.141091

O ₍₇₎	0.155852	C _(9')	-0.052437
O _(7')	0.155856	C _(10')	0.024870
		O ₍₁₁₎	0.135818

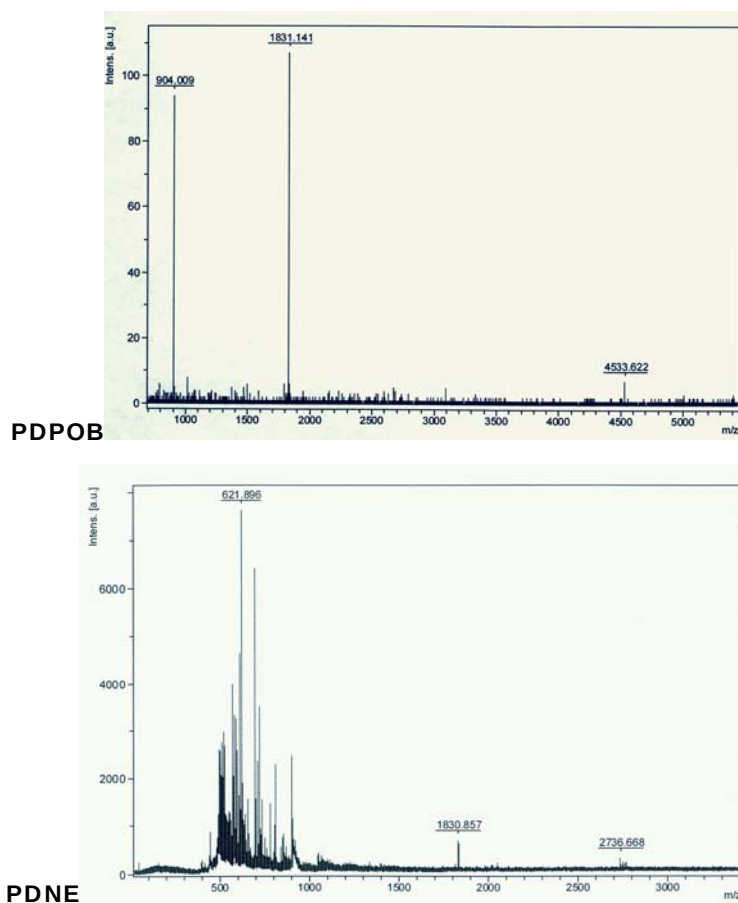


Figure S6 MALDI-TOF Mass spectra of soluble dedoped PDPOB and PDNE. Solvent: DMSO.

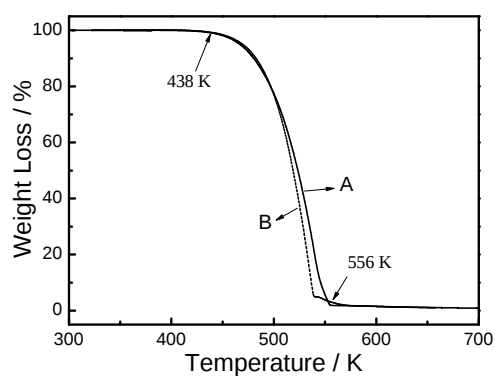


Figure S7 TGA curves of DNE (A) and DPOB (B) monomers under nitrogen protection.