Supplementary Information

Designing neurotransmitter dopamine functionalized naphthalene diimide molecular architectures for high-performance organic supercapacitor electrode materials

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Fig. S1 FT-IR spectra of NDI.



Fig. S2 ¹H NMR spectra of NDI.



Fig. S3 ¹³C NMR spectra of NDI.



Fig. S4 LR-MS spectrum of NDI.



Fig. S5 HRMS spectrum of NDI



Fig. S6 FT-IR spectra of NDI-1DP.



Fig. S7 ¹H NMR spectra of NDI-1DP.



Fig. S8 ¹³C NMR spectra of NDI-1DP.



Fig. S9 LR-MS (negative mode) spectrum of NDI-1DP.



Fig. S10 HRMS spectrum of NDI-1DP



Fig. S11 FT-IR spectra of NDI-2DP.



Fig. S12 ¹H NMR spectra of NDI-2DP.



Fig. S13 ¹³C NMR spectra of NDI-2DP.



Fig. S14 LR-MS (negative mode) spectrum of NDI-2DP.



Fig. S15 HRMS spectrum of NDI-2DP



Fig. S16 Thermogravimetric (TGA) of (a) NDI-2DP, (b) NDI-1DP and (c) NDI.



Fig. S17 Three-electrode system: Scan rate dependent cyclic voltammograms of (A) **NDI-1DP** and (B) **NDI**.



Fig. S18 Two electrode solid-state symmetric capacitor: Scan rate dependent cyclic voltammograms of (A) **NDI-1DP** and (B) **NDI**.



Fig. S19 Ragone plot for the (A) NDI-1DP and (B) NDI symmetric cell device.

Naphthale no diimido	Electrolyte	Single electrode-			CD			Cycle No.	Ref
derivatives		Volta	Scan	Cs	Voltage	Curr.	Cs	Cs (A g ⁻¹)	110.
		ge	rate	(F	(V)	Density	(F g ⁻¹)	retention	
		(V)	(mV s ⁻¹)	g-1)		(A g ⁻¹)		(%)	
TPA-1Th-	1 M TEATFB	-2.0	10		0 to 2	0.1 mA	22	500 at 0.1	1
NDI	in 1:1	to 0						mA	
	PC and DMC							>90%	
(NIBDZ)	1 M H ₃ PO ₄	0 to 1	100		0 to 1	0.5	66.56	***	2
P2	$0.5 \text{ M H}_2\text{SO}_4$	-0.7	10		-0.7 to	0.5	124	5000 at 0.5	3
P(NDI2OD		to 0.5			0.5			100%	
-									
OThCNPV)									
P1	$0.5 \text{ M H}_2\text{SO}_4$	-0.7	10		-0.7 to	0.5	84		3
P(NDI2OD		to 0.5			0.5				
-OThPV)									
P(NDI2OD	$0.5 \text{ M H}_2\text{SO}_4$	-0.7	10		-0.7 to	^a 0.5	61		3
-T2)		to 0.5			0.5				
P(NDI-Alt-	1 M PC-	-0.2	10		-1.0 to 1	^b 0.5	80		4
BDT)	LiClO ₄	to 1.1							
P(NDI-r-	1 M PC-	-2.0	5		-1.0 to	0.5	44		4
BDT)	LiClO ₄	to 2.0			1.0				
NDI-	$1 \text{ M H}_2 \text{SO}_4$	0 -	5	202.	0 to 1	0.5	195.9	10000 at 3	This
2DP/CP		1.0		5				mA cm ⁻²	work
								96 %	

Table S1. Comparison of the electrochemical performances of Naphthalenediimide derivatives with other literature.

Tetraethylammonium tetrafluoroborate (TEATFB), Propylene carbonate (PC) Dimethylcarbonate (DMC)

References

- D.F.Zeigler, S.L.Candelaria, K.A.Mazzio, T.R.Martin, E.Uchaker, S.Suraru, L.J.Kang, G.Cao and C.K.Luscombe, *Macromolecules*, 2015, 15, 5196-5203.
- 2 A. Roy, S. Mondal, A. Halder, A. Banerjee, D. Ghoshal, A. Paul and S. Malik, *Eur. Poly.* J., 2017, 93, 448-457.
- 3 S. Sharma, R. Soni, S. Kurugot and S. K. Asha, Macromolecules, 2018, 51, 954–965.
- 4 S. Sharma, R. Soni, S. Kurugot and S. K. Asha, J. Phys. Chem. C, 2019, 123, 2084–2093.