

Supplementary information

The effect of different organic solvents and anion salts on sodium ion storage in cylindrical carbon nanopores

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Table S1 Number of cations and anions inside the 4 nm region of 5 nm nanotube. .

Solvent	Electrolyte	Cation/ Anion (CNT Diameter:2 nm)	Cation / Anion (CNT Diameter: 3 nm)
EC	NaBF ₄	2.0±0.2/2.0±0.2	11.8±0.9/11.8±1.1
	NaPF ₆	2.0±0.2/2.0±0.2	11.9±0.9/12.0±1.0
	NaTFSI	4.1±0.1/4.2±0.3	9.1±0.8/10.0±1.4
PC	NaBF ₄	3.0±0.2/3.1±0.2	11.1±0.8/11.2±1.0
	NaPF ₆	1.9±0.2/2.1±0.2	10.1±0.9/10.0±1.0
	NaTFSI	4.1±0.2/4.2±0.3	9.2±0.7/10.1±1.3
EMC	NaBF ₄	4.9±0.2/5.1.0±0.2	13.0±0.9/13.1±1.1
	NaPF ₆	4.0±0.2/3.9±0.3	13.2±1.0/13.1±1.1
	NaTFSI	5.1±0.3/5.2±0.3	13.3±0.9/14.2±1.4

Table S2 Nearest neighbour distances (nm) of EC solvents, cations (Na⁺) and anions used in bulk solution (1 M) and in carbon nanotubes.

EC	EC-EC	EC-Na ⁺	EC-BF ₄ ⁻	Na ⁺ -BF ₄ ⁻
Bulk	0.23/0.31	0.23	0.37	0.34/0.85
2nm	0.23/0.31	0.23	0.39	0.34
3nm	0.23/0.31	0.23	0.38	0.34

EC	EC-EC	EC-Na ⁺	EC-PF ₆ ⁻	Na ⁺ -PF ₆ ⁻
Bulk	0.23/0.31	0.23	0.40	0.33/0.86
2nm	0.23/0.31	0.23	0.42	0.87 (shoulder)
3nm	0.23/0.31	0.23	0.42	0.42

EC	EC-EC	EC-Na ⁺	EC-TFSI ⁻	Na ⁺ -TFSI ⁻
Bulk	0.23/0.31	0.23	0.44	0.30/0.83
2nm	0.23/0.31	0.23	0.44	0.83
3nm	0.23/0.31	0.23	0.44	0.83

Table S3 Nearest neighbour distances (nm) of PC solvents, cations (Na^+) and anions used in bulk solution (1 M) and in carbon nanotubes.

PC	PC-PC	PC- Na^+	PC- BF_4^-	Na^+ - BF_4^-
Bulk	0.32	0.23	0.36	0.28
2nm	0.32	0.23	0.40	0.34
3nm	0.32	0.23	0.40	0.34

PC	PC-PC	PC- Na^+	PC- PF_6^-	Na^+ - PF_6^-
Bulk	0.32	0.23	0.41	0.33/0.86
2nm	0.32	0.23	0.45	0.41
3nm	0.32	0.23	0.45	0.41

PC	PC-PC	PC- Na^+	PC-TFSI $^-$	Na^+ -TFSI $^-$
Bulk	0.32	0.23	0.45	0.29/0.89
2nm	0.32	0.23	0.45	0.87
3nm	0.32	0.23	0.45	0.87

Table S4 Nearest neighbour distances (nm) of EMC solvents, cations (Na^+) and anions used in bulk solution (1 M) and in carbon nanotubes.

EMC	EMC-EMC	EMC- Na^+	EMC- BF_4^-	Na^+ - BF_4^-
Bulk	0.24	0.23	0.43	0.28
2nm	0.24	0.23	0.44	0.36
3nm	0.24	0.23	0.44	0.36

EMC	EMC-EMC	EMC- Na^+	EMC- PF_6^-	Na^+ - PF_6^-
Bulk	0.24	0.23	0.45	0.33/0.86
2nm	0.24	0.23	0.46	0.43
3nm	0.24	0.23	0.46	0.43

EMC	EMC-EMC	EMC- Na^+	EMC-TFSI $^-$	Na^+ -TFSI $^-$
Bulk	0.24	0.23	0.46	0.29/0.80
2nm	0.24	0.23	0.46	0.54
3nm	0.24	0.23	0.46	0.54

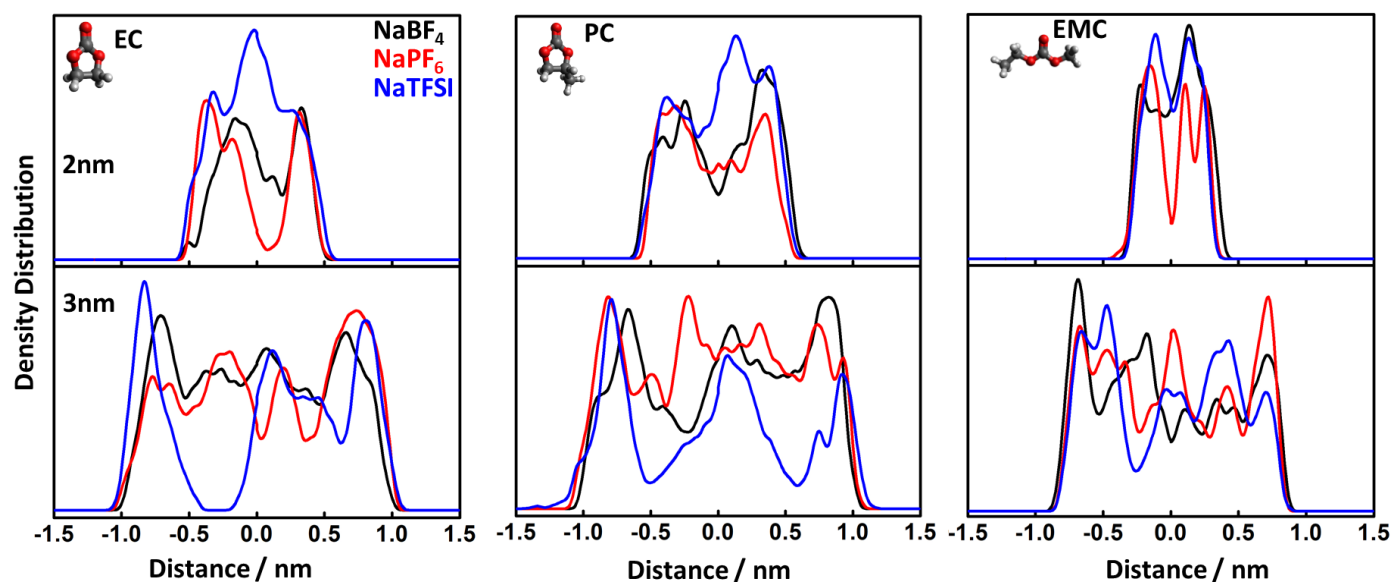


Fig. S1 Distribution of the Na^+ from the centre of the CNTs with 2 and 3 nm in presence of different anions and solvents.

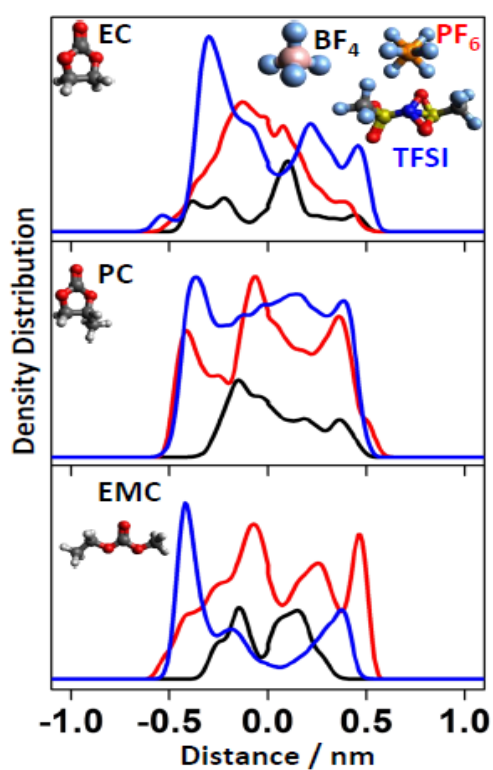


Fig. S2 Distribution of the anion in 2 nm CNTs.

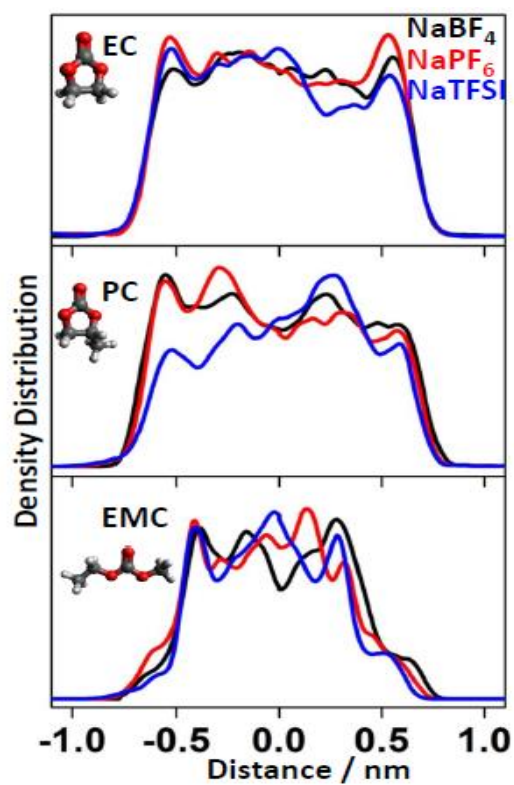


Fig. S3 Distribution of the solvent in 2 nm CNTs.

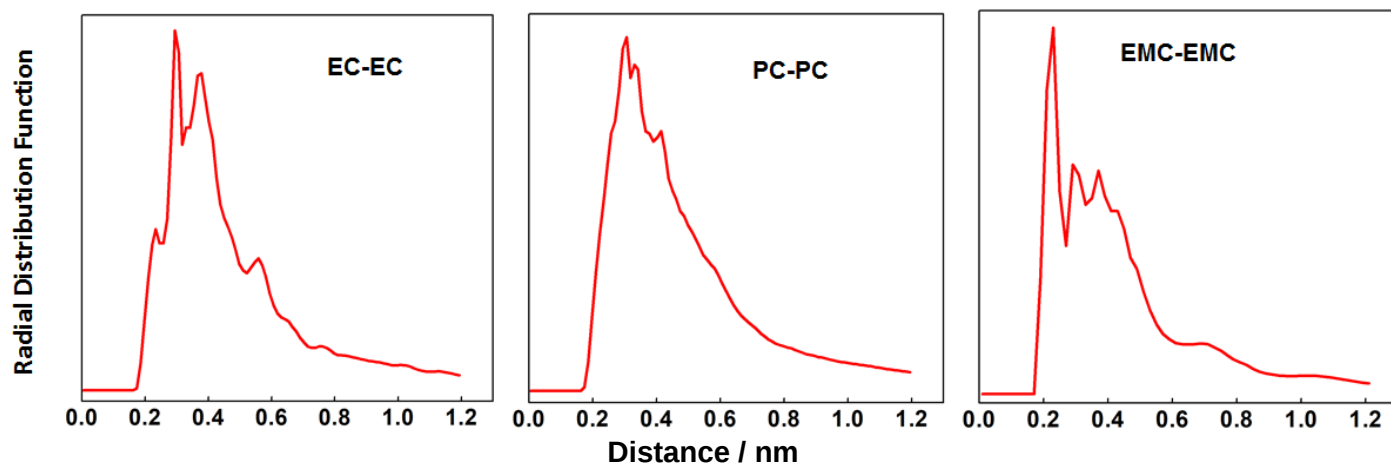


Fig. S4 Solvent-Solvent RDF inside the 1 nm CNT.