

## The effect of different organic solvents on sodium ion storage in carbon nanopores

Argyrios Karatrantos,<sup>1,2</sup> Sharif MD Khan,<sup>3</sup> Tomonori Ohba,<sup>3\*</sup> Qiong Cai<sup>1\*</sup>

1. Department of Chemical and Process Engineering, University of Surrey, Guildford GU2 7XH, UK

2. Luxemburg Institute of Science and Technology, 5, avenue des Hauts-Fourneaux, L-4362 Esch-sur-Alzette, Luxemburg

3. Graduate School of Science, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522, Japan

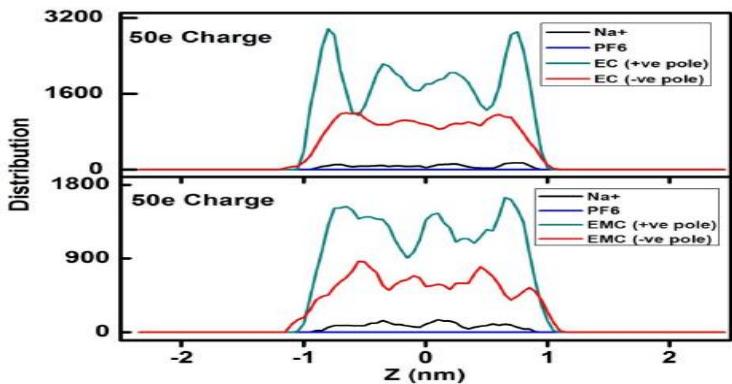
### Supplementary information

Table I: Number of the cations ( $\text{Na}^+$ ), anions ( $\text{PF}_6^-$ ) and different solvents: Ethyl Carbonate (EC), Ethyl Methyl Carbonate (EMC) and Propylene Carbonate (PC) in neutral carbon nanopores at different pore size 2, 3, 4 and 5nm.

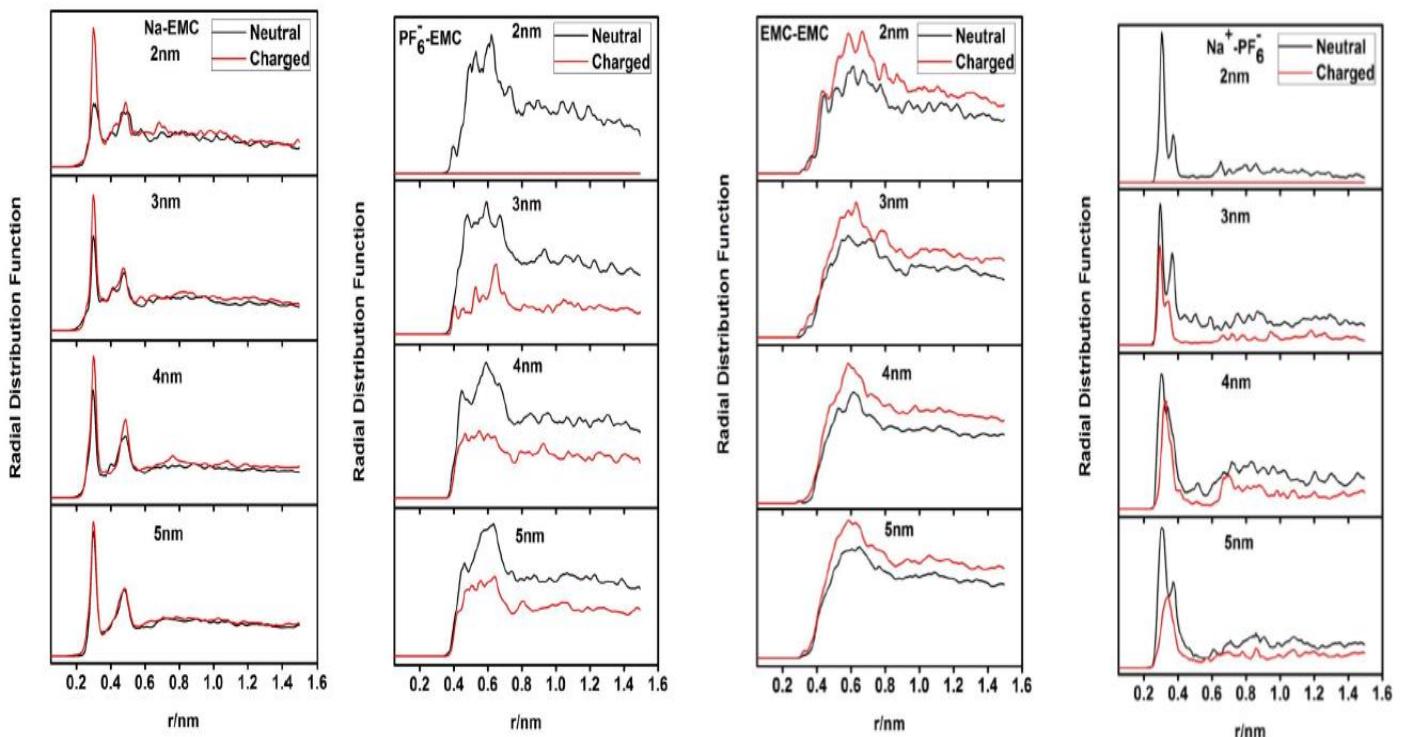
Slit width	2 nm		3 nm		4 nm		5 nm	
	Na ( $\text{PF}_6^-$ )	Solvent						
EC	30	313±22	45	474±37	60	631±51	75	780±62
EMC	30	201±13	45	311±23	60	419±40	75	525±45
PC	30	234±16	45	359±21	60	480±40	75	596±45

Table II: Number of the cations ( $\text{Na}^+$ ), anions ( $\text{PF}_6^-$ ) and different solvents: Ethyl Carbonate (EC), Ethyl Methyl Carbonate (EMC) and Propylene Carbonate (PC) in charged carbon nanopores at different pore size 2, 3, 4 and 5nm.

Slit width	2 nm			3 nm			4 nm			5 nm		
	Na	$\text{PF}_6^-$	Solvent									
EC	30	0	350±19	45	15	504±32	60	30	660±51	75	45	804±63
EMC	30	0	225±14	45	15	342±31	60	30	483±11	75	45	597±16
PC	30	0	259±15	45	15	395±30	60	30	513±40	75	45	620±41
EC	50	0										
EMC	50	0										



**Figure S1:** Density distribution along the z direction in EC, EMC. i) Carbons of EC, EMC (cyan line), ii) Carbonyl oxygen of EC, MC, iii) Na (black line), iv)  $\text{PF}_6^-$  (blue line), v)  $\text{Na-PF}_6^-$  (red line). Lines are for charged nanopores of -50e respectively.



**Figure S2:** Density distribution along the z direction in EC, EMC. i) Carbons of EC, EMC (cyan line), ii) Carbonyl oxygen of EC, MC, iii) Na (black line), iv)  $\text{PF}_6^-$  (blue line), v)  $\text{Na-PF}_6^-$  (red line). Lines are for charged nanopores of -50e respectively.