

Supporting information

Molecular insights on capacitive deionization mechanisms inside the hydrophobic and hydrophilic carbon nanotube channel electrodes

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Table S1. The Lennard-Jones force field parameters.

Atom type	σ (Å)	ϵ (kcal.mol ⁻¹)	q (e)
O/SPCE	3.166	0.1554	-0.8476
H/SPCE	-	-	0.4238
Na ⁺	2.350	0.1300	+1
Cl ⁻	4.400	0.1000	-1
C/CNT hydrophilic	3.40	0.086	-
C/CNT hydrophobic	3.40	0.0557	-
C/separating wall	3.40	0.0557	-

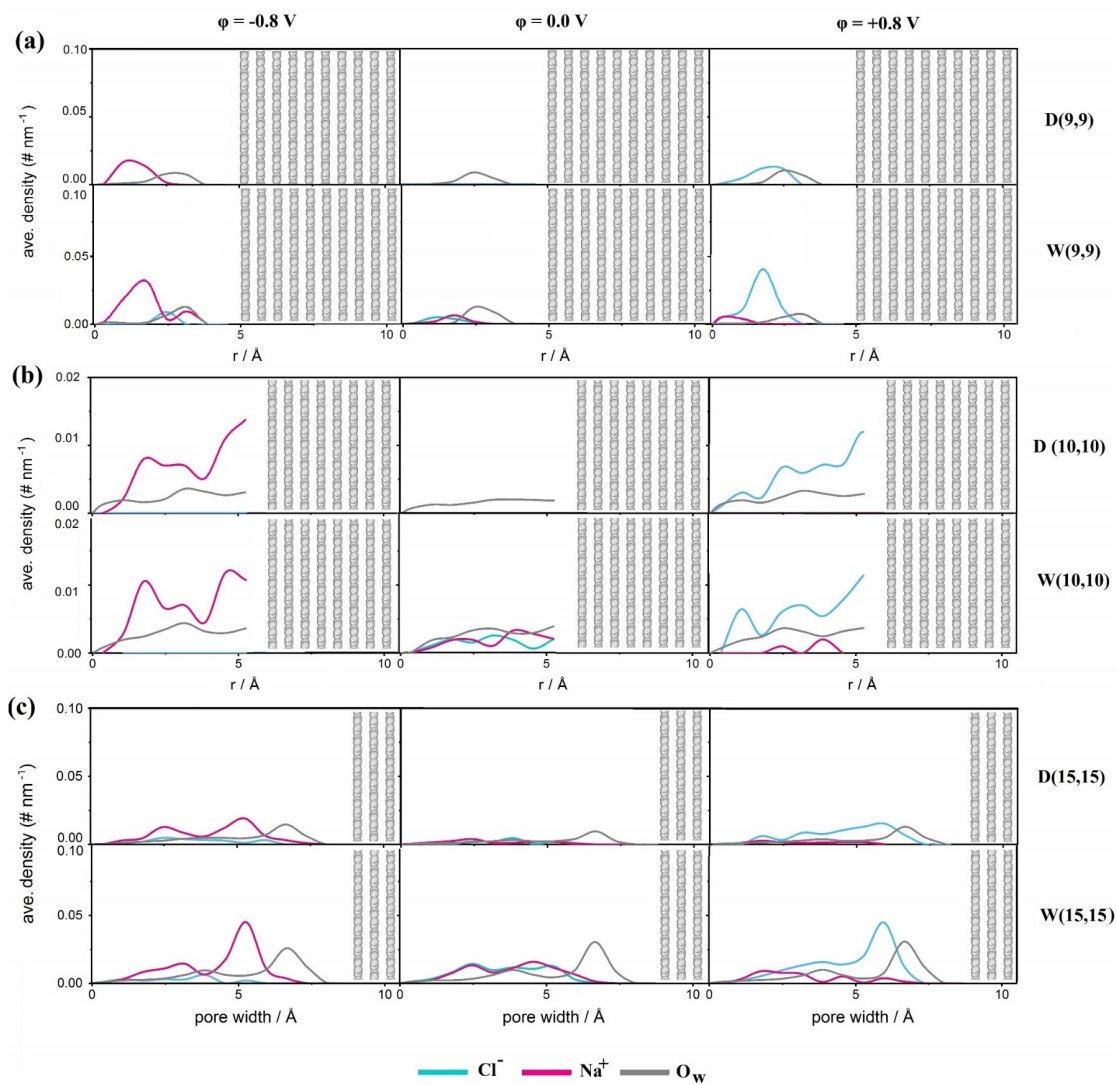


Fig. S1 The number density distribution inside the uncharged and charged electrodes (a) (9,9) (b) (10,10) (c) (15,15). The number density for oxygen was divided by 50.

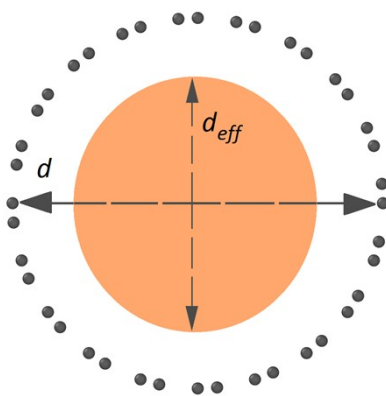


Fig. S2 The comparison of the effective diameter (d_{eff}) and the geometric diameter (d) of a CNT.

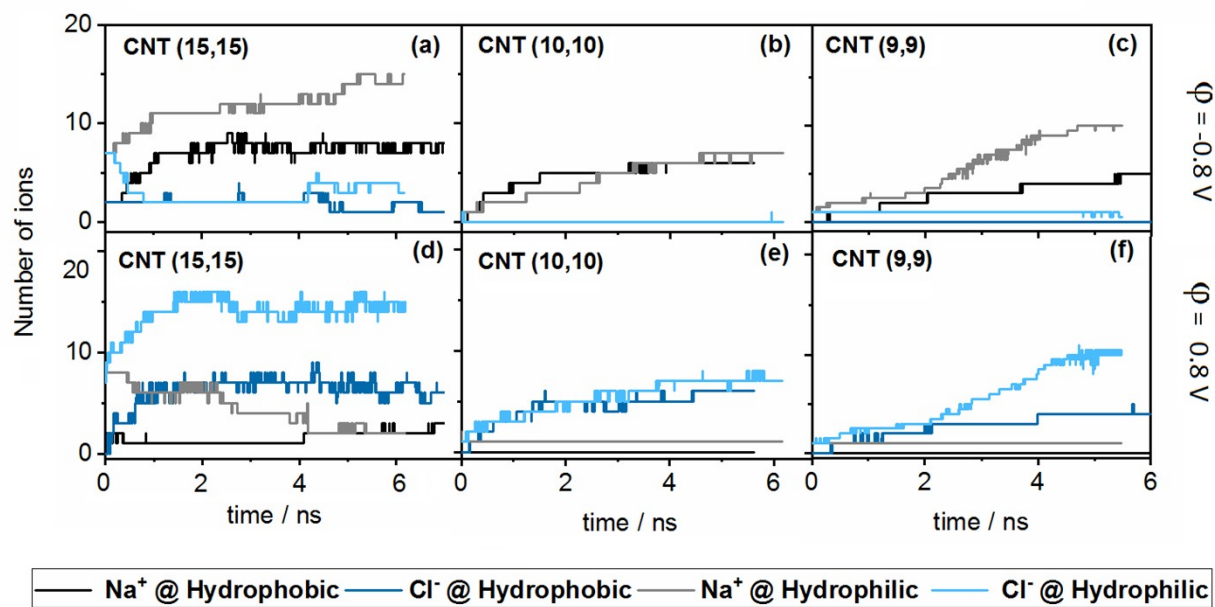


Fig. S3 The ion electrosorption/repulsion dynamic over the charging time (a) cathode CNT (15,15) (b) cathode CNT (10,10) (c) cathode CNT (9,9) (d) anode CNT (15,15) (e) anode CNT (10,10) (f) anode CNT (9,9).

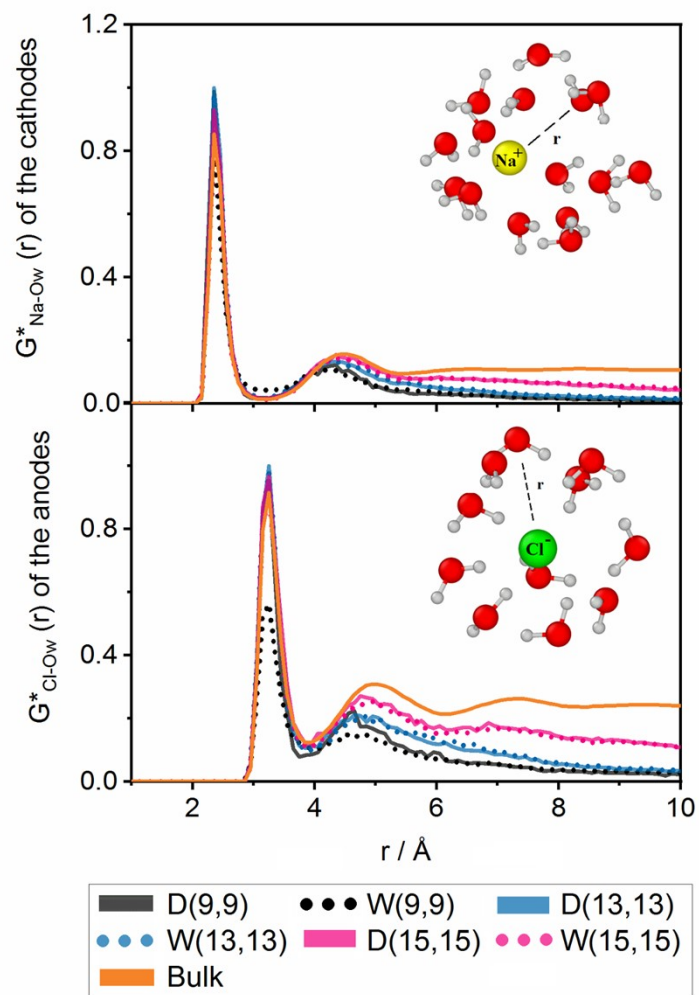


Fig. S4 The relative bulk and confined ionic species' solvation shell.

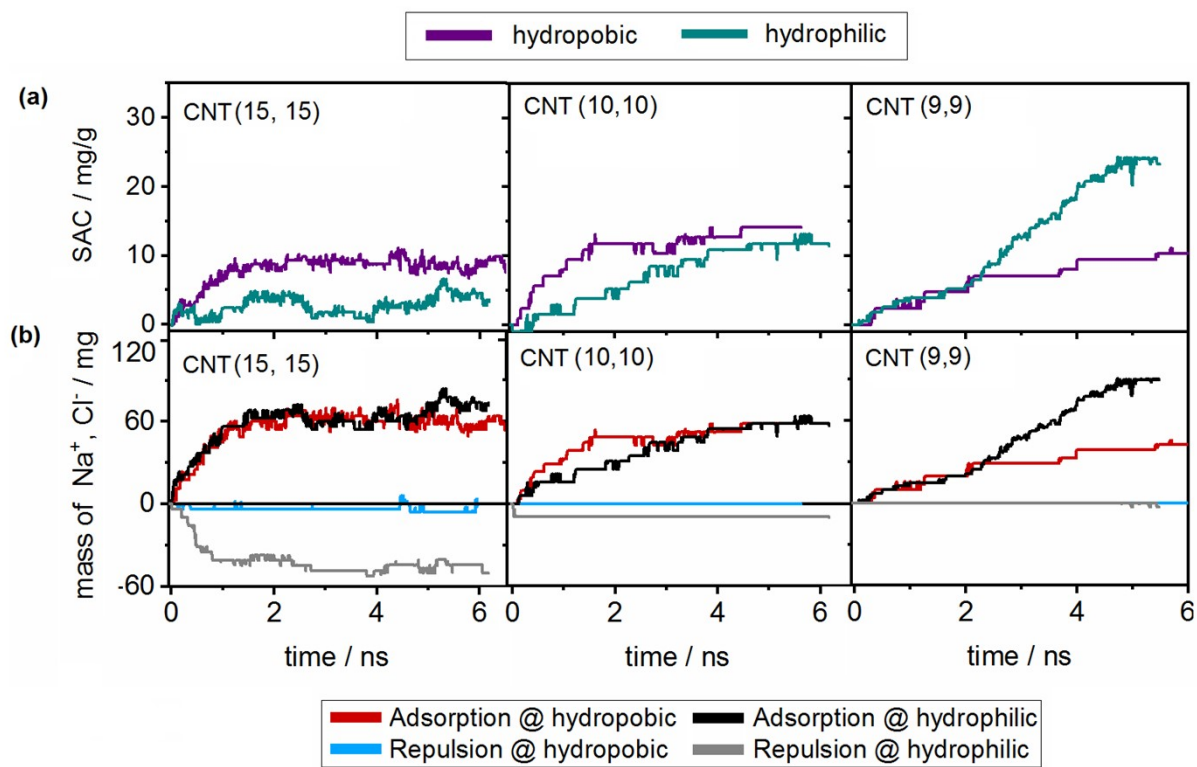


Fig. S5 (a) SAC of the CDI systems over the charging time (b) temporal mass of the in-pore ions over the charging time.

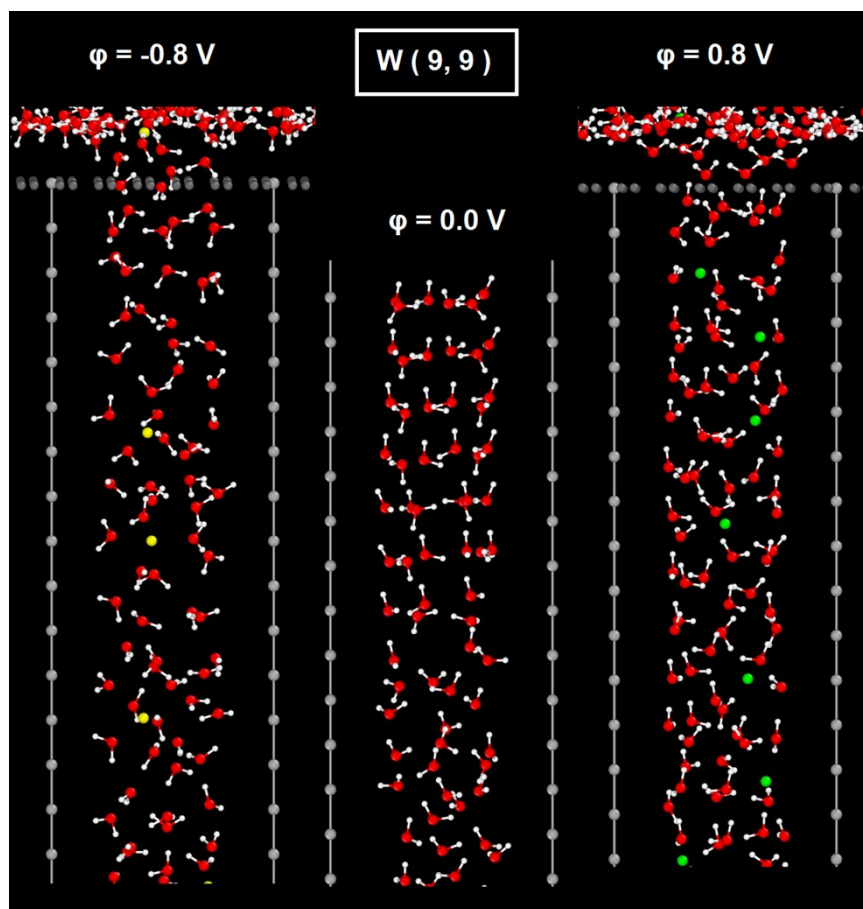


Fig. S6 The schematic showing the structure of the confined electrolyte inside the charged and uncharged W (9,9) electrodes. The white, red, yellow, green, and grey spheres represent H for water, O for water, Na^+ , Cl^- , and carbon for the electrode respectively.

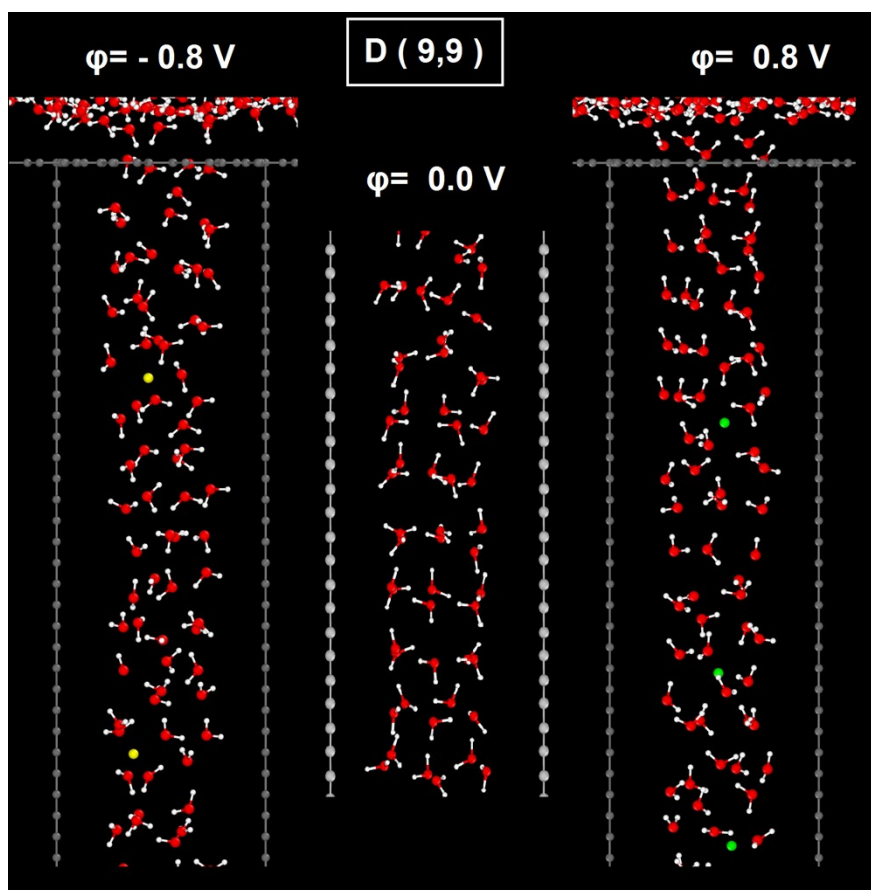


Fig. S7 The schematic showing the structure of the confined electrolyte inside the charged and uncharged D (9,9) electrodes. The white, red, yellow, green, and grey spheres represent H for water, O for water, Na^+ , Cl^- , and carbon for the electrode respectively.

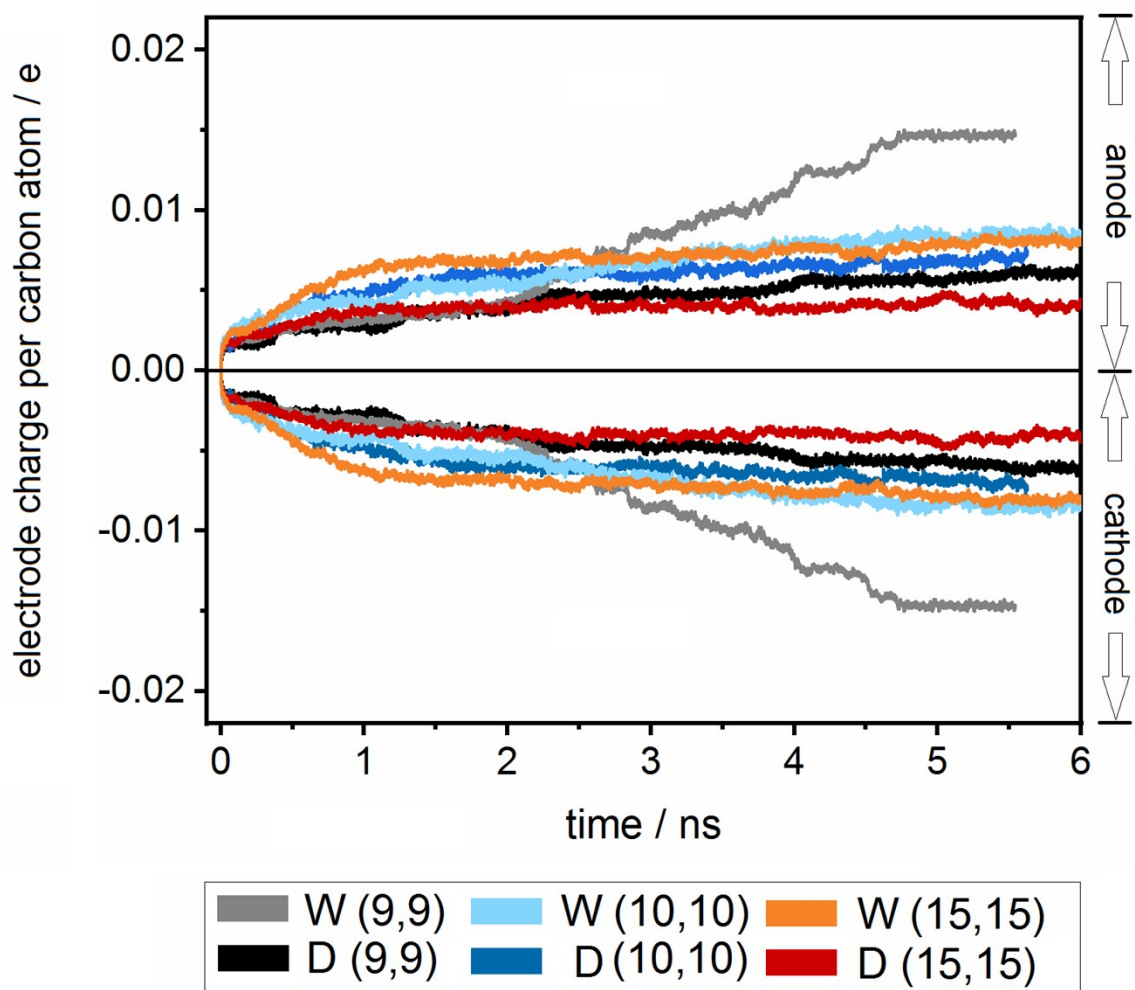


Fig. S8 Evolution of the CNT electrodes' average electronic charge per atom. The curves with positive (negative) electronic charge belong to the anodes (cathodes).

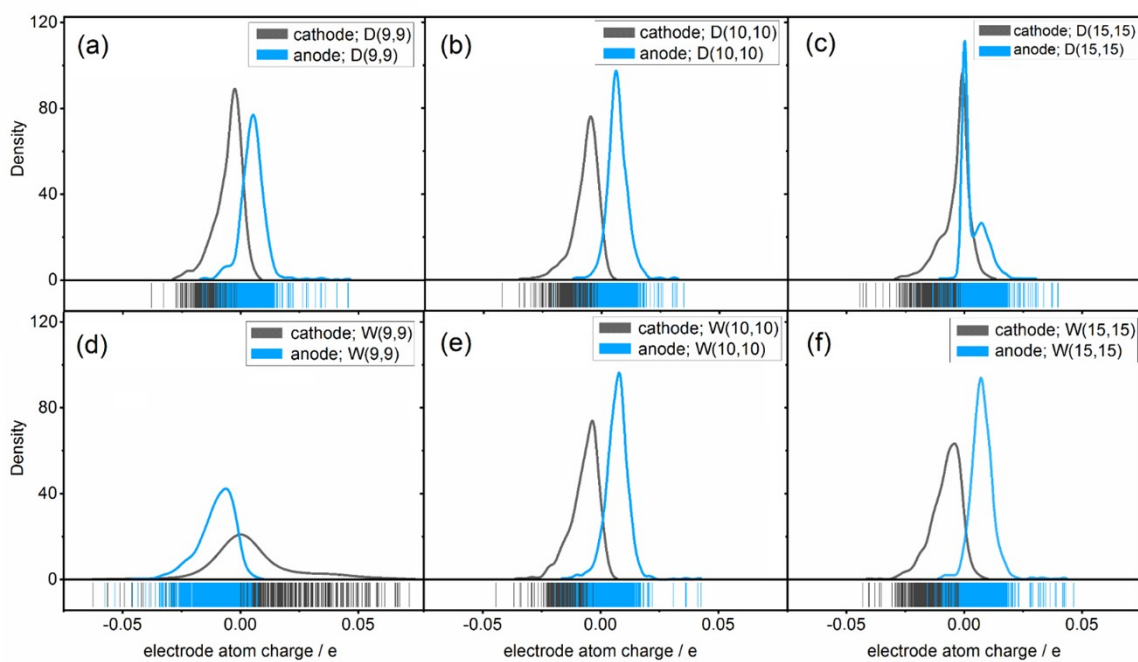


Fig. S9 The electronic charge distribution of the electrode atoms (a) D (9,9) (b) D (10,10) (c) D (15,15) (d) W (9,9) (e) W (10,10) (f) W (15,15)