Confinement, desolvation and electrosorption effects on the diffusion of ions in nanoporous carbon electrodes

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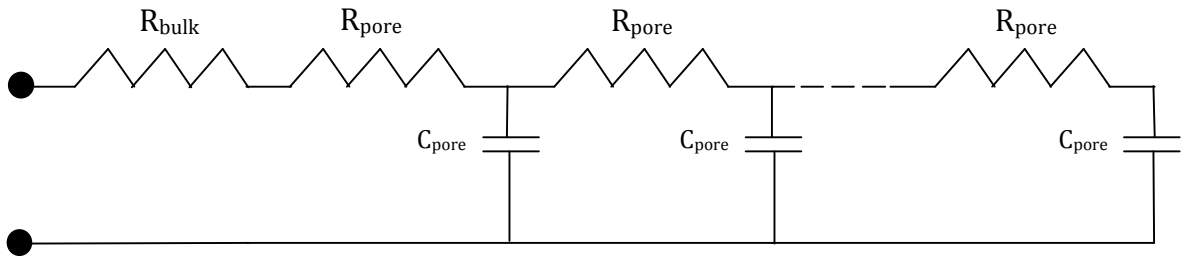
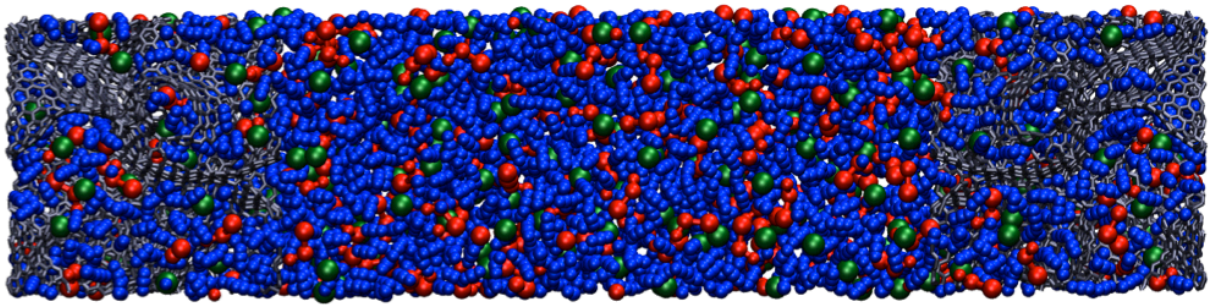
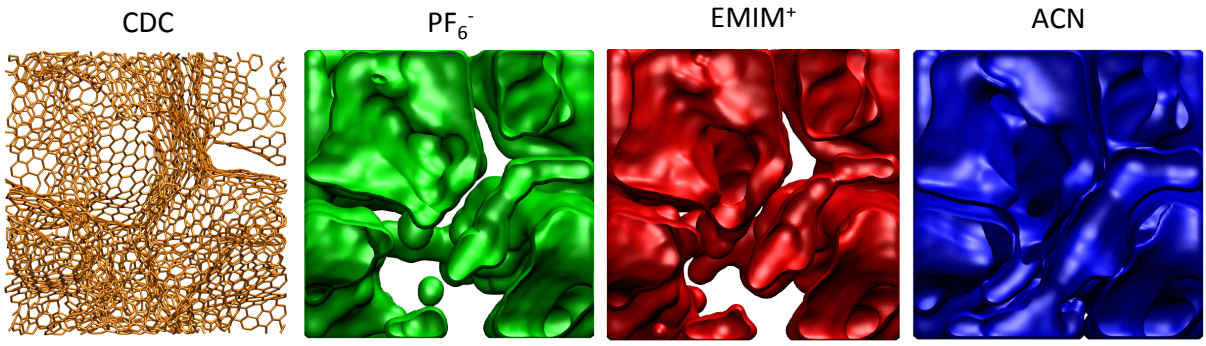
Supporting Information



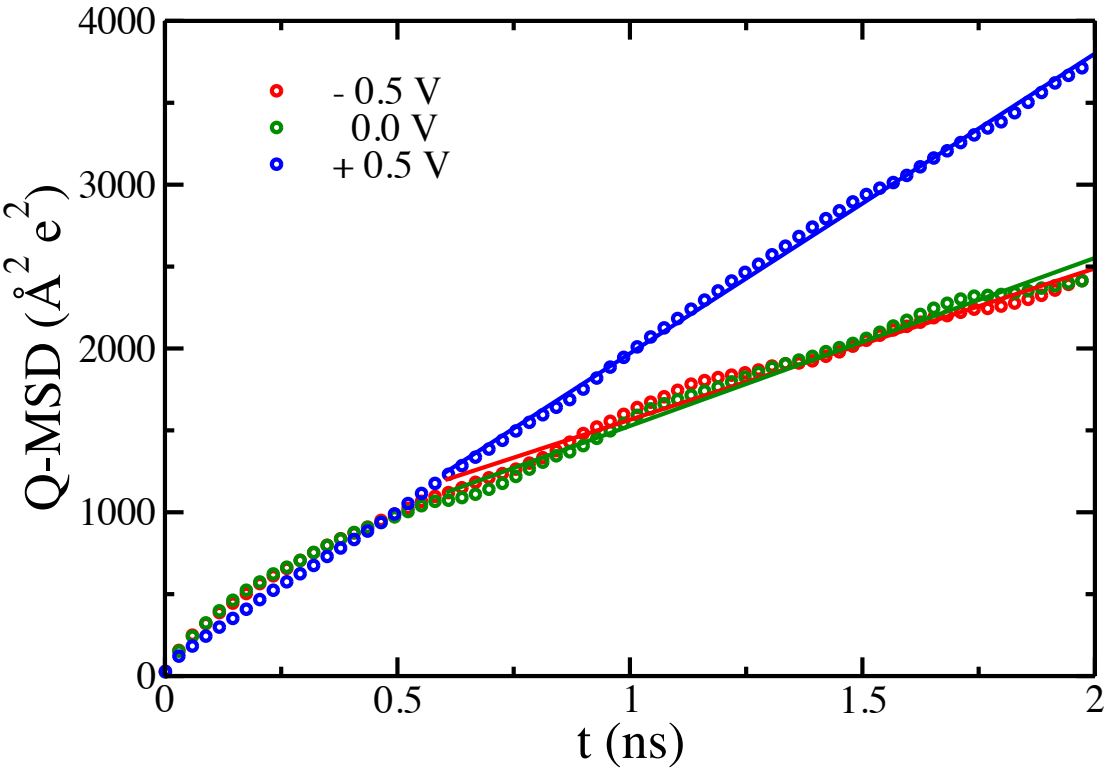
Supplementary Figure S1 : Equivalent circuit (transmission line model) of a porous carbon electrode. The bulk electrolyte is represented by the resistance R_{bulk} while the electrodes are represented by an infinite series of resistances R_{pore} and capacitors C_{pore}.



Supplementary Figure S2. The simulation cells consist of an electrolyte surrounded by two porous carbon electrodes. The electrolyte is a 1.5 M solution of BMIM-PF_6 dissolved in acetonitrile) and the porous carbon mimics a carbide-derive carbon with an average pore size of 0.9 nm. The lateral dimension of each electrode is of 4.4 nm, while the distance between them is 24 nm. Anions are colored in green, cations in red, acetonitrile in blue and carbon atoms in gray.



Supplementary Figure S3 : Accessible volume for the electrolyte species inside the electrodes. Volumetric representation of the positions which have been occupied by the center of mass of each molecule type during our simulations.



Supplementary Figure S4 : The plotted quantity is the sum in the right-hand term of Equation 3. The in-pore conductivities are extracted from the linear régime (shown using straight lines).