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Supercapacitors with lithium-ion electrolyte: an experimental study and design of the activated carbon electrodes via modelling and simulations

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INPUT DATA FOR THE ELECTROLYTE

Table SI-1. Values of parameters and properties of the electrolyte system used in the simulations of this study.

Electrolyte **1 M $LiPF_6$ /EC:EMC at 50:50 v/v**	
Dissociation constant, k_d	1. [calculated in this study to match σ_2]
Deformed "flat" solvated Li in small micropores: d_{Li+} (nm) $d_{Li+,min}$ (nm) $d_{Li+,max}$ (nm)	 0.56 0.56 1.527
V_{Li+} (nm^3)	0.092
Desolvated PF_6-: d_{PF6-}(nm) $=d_{PF6-,min}=d_{PF6-,max}$	 0.5 [1]
V_{PF6-} (nm^3)	0.069 [1]
Solvated tetrahedral Li^+/EC:EMC: $d_{Li+/EC:EMC}$ (nm) $d_{Li+/EC:EMC,min}$ (nm) $d_{Li+/EC:EMC,max}$ (nm)	 1.8 [2] 1.8 [2] 1.93 [2]
Solvated PF_6/EC:EMC: $d_{PF6-/EC:EMC}$ (nm) $=d_{PF6-/EC:EMC,min}$	 1.4 [1,2]

$=d_{PF6-/EC:EMC,max}$	
$E_{Li+/EC:EMC}$ (kJ/mol)	-400 [3]
$n_{Li+/EC:EMC}$	4 [2]
Desolvation: $\Delta n_{Li+/EC:EMC}$	0
$E_{PF6-/EC:EMC}$ (kJ/mol)	-70 [4]
$n_{PF6-/EC:EMC}$	3 [2]
$\Delta n_{BF4-/AN}$	3
Dielectric constant of solvent, ε_r	52 [5]
Solvent viscosity η_o (mPa s)	1.4 [5]
Conductivity σ_2 (S m^{-1})	0.5

Solvent viscosity and dielectric constant were obtained from the cited papers, which reported the properties of single solvents and solvent mixtures at different ratio to 50:50 v/v employed in this study: those values were then interpolated to the solvent mixture composition of this study by following a simple rule of mixtures. The conductivity of the electrolyte was calculated using equations (6-8) and (10) of the main manuscript, where the electrolyte dissociation constant was fitted to $k_d = 1$, so that the conductivity of the electrolyte is correctly related to R_1 value in Table 1 for this electrolyte and also in relation to the R_1 values for the other EDLCs with the two other electrolytes in Table 1, for which their conductivity values were also known.

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