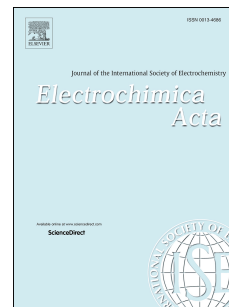


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## Electrolyte Cation Length Influences Electrosorption and Dynamics in Porous Carbon Supercapacitors

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### Abstract

We investigate the extent to which the alkyl chain on the cation of an imidazolium-based neat room-temperature ionic liquid influences mobility and electrochemical behavior in nanoporous supercapacitors. Changing the cation chain length from an ethyl ( $n = 2$ ) to a butyl ( $n = 4$ ) to a hexyl ( $n = 6$ ) group affects the electrolyte dynamics and their accumulation densities under dynamic charge-discharge processes. We relied on molecular dynamics (MD) computational simulations and classical density functional theory (cDFT) calculations of our system to reinforce the experimental results obtained from electrochemical measurements and quasi-elastic neutron scattering (QENS). We contrast the different dynamics of ionic liquids in bulk and confined states and demonstrate the effect of the cation dimension on resulting arrangements of positive and negative ions in pores. We correlate these fundamental properties with device performance metrics in an effort to properly tailor high-performance carbon supercapacitor electrodes with non-flammable and electrochemically stable electrolytes.

**Keywords:** supercapacitor; ionic liquid; molecular dynamics; density functional theory; neutron scattering

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