Ion mobility studies in model carbons by solid state MAS- and *In-Situ*-NMR spectroscopy

N. Fulik[1*], **F. Hippauf**[2], **D. Leistenschneider**[2], **E. Zhang**[2], **L. Borchardt**[2], **S. Paasch**[1], **S. Kaskel**[2], **E. Brunner**[1]

[1] Technische Universität Dresden, Institute of Bioanalytical Chemistry, Dresden, Germany
[2] Technische Universität Dresden, Institute of Inorganic Chemistry I, Dresden, Germany
[*]nataliafulik@gmail.com

Electrical Double Layer Capacitors (EDLC, also denoted as supercapacitors) are important energy storage devices, especially to rapidly store or deliver high amounts of electrical charge. Their energy storage principle is based on the formation of electrical double-layers and depends strongly on the electrode surface as well as other parameters.[1,2] The understanding of the molecular processes in EDLCs are crucial for better design. In the present contribution, we investigate the ion mobility in carbon electrode materials loaded with electrolyte solutions by solid-state NMR spectroscopy.

Well-defined carbon materials of known porosity such as the purely microporous carbide-derived carbon TiC-CDC1000, mesoporous carbon CMK-3 and micro/mesoporous carbide-derived carbon OM-CDC are used in our model studies. These samples were chosen in order to elucidate the influence of the different pores upon the mobility of the electrolyte constitutes. The samples are loaded with well-defined amounts of 1M tetraethylammonium tetrafluoroborate ($TEABF_4$) in deuterated acetonitrile. Solid-state NMR-Spectroscopy is capable of studying host-guest interactions in these electrolyte-loaded carbon materials. ^{11}B, ^{1}H and ^{2}H MAS NMR spectroscopy allows to discriminate between the different electrolyte constituents. Line shape analysis of 1D spectra and 2D EXSY NMR spectroscopy allow to derive the characteristic time scale for processes such as the intra-particle exchange between different pores inside the carbon particle, the exchange between the pore system and the surrounding bulk, and the inter-particle exchange.

In addition to the MAS NMR experiments, the model carbons were also processed into supercapacitors and studied by *in situ* ^{11}B NMR spectroscopy in analogy to experiments performed on commercial supercapacitors by the Grey group[4] and compared with the results of cyclovoltammetric measurements obtained on the same samples. In summary, it could be shown that the presence of well interconnected micro- and mesopores as found in OM-CDC results in a high mobility of the electrolyte ions combined with a very high internal surface area, i.e., high capacitance. The ion high mobility is favorably influences the behavior of the supercap in rapid charge/discharge cycles.

References

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