QUANTITATIVE NANO-STRUCTURE-PROPERTY RELATIONSHIPS OF NANOPOROUS CARBON

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Nanoporous carbon materials play a major role in modern industry. They are widely used in energy storage devices such as batteries, supercapacitors and fuel cells due to their large surface area and high surface to volume ratio [1]. Studying the relationships between the porous structure and energy storage behaviour of carbon materials is one possible approach in order to develop further electrical double-layer based supercapacitors.

In this study [2], 100 carbide-derived carbon (CDC) materials, synthesized via chlorination of different metal carbides at variable reaction conditions, were experimentally characterized. Porosity characteristics (experiment-derived nano-molecular descriptors) of CDC samples were determined by low-temperature N_2 adsorption. The electrochemical characteristics, cathodic and anodic capacitances in a nonaqueous electrolyte (TEMA-BF_4 in propylene carbonate), were calculated at 5 mA cm^{-2} from the constant current discharge (CCD) experiments at the potential ranges of 0 to −1.4 V and 0 to +1.4 V, respectively. These data were analysed and modelled using the Quantitative nano-Structure Property Relationship (QnSPR) approach.

The analysis and modelling shows that the QnSPR approach provides a useful tool to describe and predict various performance-related physical properties of nanoporous carbon. As a main result, a three-parameter QnSPR model describing the volumetric cathodic capacitance of CDC by specific surface area, volume of a certain pore size fraction and a density of carbon electrode was developed.

References

1. Supercapacitors: Materials, Systems, and Applications; Béguin, F., Frąckowiak, E., Eds.; Materials for sustainable energy and development; Wiley-VCH: Weinheim, 2013.
2. M. Käärik, U. Maran, M. Arulepp, A. Perkson, J. Leis, Quantitative nano-structure–property relationships for the nanoporous carbon: predicting the performance of energy storage materials, ACS Appl. Energy Mater. 1 (2018) 4016–4024.

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