Combining Water, Argon, and Nitrogen Adsorption for an Advanced Characterization of Nanoporous Carbons

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During recent years, major progress has been achieved in the understanding of the adsorption and phase behavior in ordered micro- and mesoporous materials with simple pore geometries, which has led to major advances in the structural characterization by physical adsorption. However, the effects of geometrical and chemical heterogeneities of the pore walls on the sorption, phase, and wetting behaviors of fluids in nanoporous materials such as nanoporous carbons are still under investigation. Within this context, the potential use of water as a probe for surface chemistry and pore structure characterization of nanoporous carbon materials has led to a lot of interest. The use of water adsorption is attractive because it can be performed at room temperature, water has a very small kinetic diameter which allows it to enter pores even smaller than the ones accessible to carbon dioxide, argon, nitrogen and it is sensitive to surface chemistry. On the other hand, the interpretation of water adsorption data is not straightforward, mainly because details of the water adsorption isotherms are strongly affected by both pore structure and surface chemistry and the underlying mechanism of water adsorption in nanoporous carbons is still under investigation. Also, the majority of the water adsorption studies reported so far have been performed on fairly disordered porous carbon materials (e.g. activated carbon fibers, activated carbon. Hence, in order to further assess the potential of water adsorption for textural and surface characterization, we have performed a systematic, physical adsorption characterization which includes activated carbons, but also ordered micro/mesoporous carbons (CMK-1, CMK-3, CMK-8) by combining N2 (77.4K), Ar (87K) and water adsorption (over a temperature range from 293 – 313 K). An accurate micro/mesopore size analysis is obtained from the nitrogen and argon adsorption data by applying dedicated DFT methods, i.e. NLDFT (non-local density functional theory) and novel QSDFT (quenched sold density functional theory) which takes into account the effects of surface heterogeneity/roughness on nitrogen and argon adsorption .

The analysis of our water adsorption data obtained for these ordered nanocarbons in combination with nitrogen and argon adsorption (coupled with QSDFT pore size analysis) sheds light into the mechanisms of water adsorption and clearly demonstrates the potential of water as a powerful, complimentary adsorptive for the physical adsorption characterization of nanoporous carbons.