Porous Carbon Characterization Experiment and Theory: Top Down and Bottom Up

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Porous carbons are widely used for a variety of adsorption applications, including protection from chemical and biological warfare agents. Experimental characterization of these materials faces a number of challenges, such as determining: (a) the distribution of carbon microcrystal sizes; (b) the densities and species of surface groups; (c) the topological nature of the connected pore structure; and (d) pore size distributions. We represent results from combined experiment and theory, in an attempt to both characterize porous carbons used for filtration media (e.g. base BPL and ASZM-TEDA carbon) and understand the adsorption process. Experimental methods include X-ray diffraction, DRIFT, and Boehm titration. Concurrent molecular modeling is underway using the results of this experimental data to develop improved activated porous carbon models to analyze this problem in atomistic detail. Modeling techniques used include hybrid reverse Monte Carol methods, as well as molecular dynamics and ab initio and density functional quantum chemistry.