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On the characterization of nanoporous carbons with small-angle scattering

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Small-angle scattering of X-rays (SAXS) has long been used to characterize nanoporous materials. An advantage is that SAXS is sensitive to both, open and closed pores, and can thus deliver complementary information to gas sorption analysis (GSA). While integral parameters such as the specific pore volume or the specific surface area can readily be obtained from both methods using classical approaches, pore size distributions (PSDs) derived from the two techniques - even when comparing fully open pore systems - are usually hardly comparable on a quantitative level. Apart from the inherent difficulty of defining a "smooth"surface for, e.g., micropores with sub-nanometer pore sizes, also the shape and pore arrangement influences the results of a PSD determination. Here we show an attempt to make PSDs derived from SAXS and GSA data from a series of microporous activated carbons directly comparable [1]. To this end, a real space model of the pore structure is created from the SAXS data using the concept of Gaussian random fields. From these data, "size distributions", e.g., the distribution of normal distances from points on the surface to the opposite surface of a pore can easily be calculated. This distribution however deviates considerably from the PSD obtained from GSA data using a mixed quenched solid density functional (QSDFT) kernel due to its inherent assumption of slit like pores. A "Degree of Confinement"parameter accounting for the local pore geometry is employed to determine an alternative size distribution for purely slit like pores from the SAXS model, which shows good agreement with the corresponding GSA data. Potential applications of the approach may particularly be helpful for closed pore systems such as non-activated hard carbons.
References:
1. C. Prehal, S. Grätz, B. Krüner, M. Thommes, L. Borchert, V. Presser, O. Paris, Comparing pore structural models of nanoporous carbons obtained from small-angle scattering and gas adsorption, Carbon, 152 (2019) 416-423

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