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Topological defects in model nanoporous carbon: population, structural characterizations and adsorption properties XI MI, JEREMY PALMER, JORGE PIKUNIC, KEITH GUBBINS, YUNFENG SHI — Nanoporous carbon materials have drawn substantial research interests because of their unique capabilities to mediate the mass-transport, uptake through adsorptions and catalyze chemical reactions of the guest species. All aforementioned properties depend sensitively on the structural characteristics of the nanoporous carbon, including hybridization state of carbon, presence of functional groups, topology of carbon rings and curvature/connectivity of graphene sheets. Among all these defects, carbon pentagons are of particular interests since they possess 108° C-C-C bond angles which are dramatically different from the 120° angles typical for carbon hexagons and larger carbon rings. However, the pentagon concentration in the bulk has not been determined. Here we use a realistic nanoporous carbon model proposed recently to systematically synthesize a large number of samples with different concentrations of carbon pentagons using molecular simulation methods. We evaluate the different porous structures in terms of their deviations in s(q) from experiments so as to estimate pentagon concentrations. Moreover, the porous structures are related to the adsorption properties through simulated argon adsorption tests.

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