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Development and application of an advanced percolation model for pore network characterization by physical adsorption

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Physical adsorption is one of the most widely used techniques to characterize porous materials because of being reliable and able to assess micro- and mesopores within one approach. However, challenges and open questions persist in characterizing disordered and hierarchically structured porous materials. This study introduces a pore network model aiming to enhance the textural characterization of nanoporous materials. Our model, based on percolation theory on a Bethe lattice, includes all mechanisms known to contribute to adsorption hysteresis in mesoporous pore networks during capillary condensation and evaporation. The model accounts for delayed and initiated condensation during adsorption as well as equilibrium evaporation, pore blocking and cavitation during desorption. Coupled with dedicated non-local-density functional theory (NLDFT) kernels, the proposed method provides a unified framework for modeling the entire experimental adsorption-desorption isotherm, including desorption hysteresis scans. Hence, this model unveils key pore network characteristics like the effective connectivity, but also has the potential to determine pore size distributions of mesoporous materials by taking quantitatively pore network effects into account.
The applicability of the method is demonstrated on a selected set of nanoporous silica materials exhibiting distinct types of hysteresis loops (types H1, H2a, H1/H2a and H5), including ordered mesoporous silica networks, i.e, KIT-6 silica, hybrid SBA- 15/MCM-41 silica with plugged pores, but also two disordered silica pore networks, i.e., a hierarchical meso-macroporous monolith and porous Vycor glass. For all materials, good correlation is found between calculated and experimental primary adsorption and desorption isotherms as well as desorption scans allowing for a determination of key pore network characteristics such as pore connectivity and pore size distributions as well as a parameter correlated with the impact of pore network disorder and corresponding effects on the adsorption behavior. The versatility and enriched textural insights provided by the proposed novel network model allows for a comprehensive characterization previously inaccessible, and hence will contribute to a further advancement in the textural characterization of novel nanoporous materials. It has the potential to provide important guidance for the design and selection of porous materials for optimizing various applications, including separation processes (such as chromatography), heterogeneous catalysis, gas-and energy storage. [1]

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