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On the Mechanism of Water Adsorption in Carbon Micropores

A Molecular Simulation Study

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Abstract

Water adsorption in carbon micropores is of great practical interest because of its negative impact on the performance of carbonaceous adsorbents and because of the application of water as a molecular probe to characterize porous materials. The subject has also attracted much attention from theoreticians in the adsorption science community because of its unique adsorption behavior in contrast to that of simple gases. Here we have carried out a comprehensive Monte Carlo simulation to investigate the effects of functional group density, pore size and temperature on the adsorption of water in slit-like carbonaceous pores. The nucleation of water clusters, their growth and coalescence are the critical steps for water adsorption, and they have been studied over a wide range of conditions. We find that the transition from water clusters with a convex interface to ones with a concave interface, brought about by the coalescence of adjacent clusters, is the microscopic origin for hysteresis in water adsorption-desorption isotherms. We also find that the balance between energy and entropy, which changes in favor of entropy with increasing temperature, governs the onset of condensation and evaporation and hence the hysteresis observed in some isotherms.