COMPUTATIONAL STUDIES OF METHANE ADSORPTION IN NANOPOROUS CARBON

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ABSTRACT

In this thesis we have completed computational studies using Grand Canonical Monte Carlo on the adsorption of methane into a graphitic nanoporous adsorbent with slit-shaped pores. Simulations were done at a temperature of 303 K (room temperature), for pores between 7 and 50 A, and pressures from 0 to 360 bar. We identified the presence of multi-layer adsorption at supercritical temperatures with excess amount even at large distances from the pore walls. We also show that, based on pore-size distributions obtained from nitrogen adsorption, we can successfully model the experimental adsorption isotherms and isosteric heats of adsorption of methane in activated carbon.