Theoretical Modeling of n-Alkane Adsorption on Different Porous Materials using the SAFT-FMT-DFT Approach

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In this work, a theoretical approach that combines elements of the statistical associating fluid theory (SAFT), fundamental measure theory (FMT), and classical density functional theory (DFT) to create a framework to model fluids in the presence of external fields. The SAFT-FMT-DFT approach is used to calculate single pore isotherms to develop a pore size distribution different porous materials, described by the 10-4-3 fluid-wall potential, based on nitrogen adsorption at 77 K. The pore size distribution is then used to predict excess adsorption isotherms for alkanes. The predicted isotherms are found to be in good agreement with the experimental data.