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Modeling Adsorption of Simple Fluids and Alkanes on 3D Nanoporous Carbons

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Predicting adsorption on nanoporous carbonaceous materials is important for developing various adsorption and membrane separations, as well as for oil and gas recovery from shale reservoirs. Here, we explore the capabilities of 3D molecular models of disordered carbon structures to reproduce the morphological and adsorption features of practical adsorbents. Using grand canonical Monte Carlo simulations, we construct a series of adsorption isotherms of simple fluids (CO2, N2, and SO2) and a series of alkanes from methane to hexane on two model 3D structures: purely microporous structure A and micro-mesoporous structure B. We show that structure A reproduces the morphological properties of commercial Norit R1 Extra activated carbon and demonstrates outstanding agreement between the simulated and experimental adsorption isotherms reported in the literature for all adsorbates considered. Good agreement is also found for simulated and measured isosteric heats. This work provides a new insight into the specifics of structural and adsorption properties of nanoporous carbons and demonstrates the advantages of using 3D molecular models for predicting adsorption hydrocarbons and other chemicals by MC simulations.
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Primary authors: CORRENTE, Nicholas (Rutgers University); HINKS, Elizabeth (Rutgers University); KASERA, Aastha (Rutgers University); GOUGH, Raleigh (Rutgers University); RAVIKOVITCH, Peter I. (ExxonMobil Research and Engineering Company); NEIMARK, Alexander (Rutgers University, New Jersey, USA)

Presenter: CORRENTE, Nicholas (Rutgers University)

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