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SAFT-DFT Studies of Nanoporous Carbon Deformation Induced by Multicomponent Adsorption

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We consider deformation of nanoporous carbons during adsorption of mixtures, focusing on the specific context of carbon dioxide displacement of natural gas from coal and shale reservoirs. Density functional theory calculations augmented by the perturbed chain statistical associating fluid theory (SAFT-DFT) are employed to model adsorption of fluid mixtures on carbon slit pores at geologically relevant temperatures and pressures. The adsorption stress is calculated from the change in the grand thermodynamic potential of the adsorbed fluid with respect to the change in pore volume. Adsorption of methane and carbon dioxide mixtures is studied in pores of various size. We determine the effect of pore size and fluid composition on the adsorption-induced deformation. The results of this method show good agreement with atomistic GCMC simulations at a fraction of the computational cost.
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Primary authors: CORRENTE, Nicholas (Rutgers University); HINKS, Elizabeth (Rutgers University); KASERA, Aastha (Rutgers University); NEIMARK, Alexander (Rutgers University, New Jersey, USA)

Presenter: CORRENTE, Nicholas (Rutgers University)

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