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3-D Density Functional Theory to Describe Adsorption of Pure Substances and Their Mixtures on Crystalline and Amorphous Adsorbents

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The 1-D, 2-D, and 3-D classical Density Functional Theory (cDFT) consistent with the PC-SAFT equation of state are used to investigate the adsorption isotherms and local densities of pure hydrocarbons, H₂, and CO₂ and their mixtures in crystalline-structure materials (like MOF-5) and amorphous materials (like nanoporous carbons). The cDFT calculations reveal that the adsorption process is influenced by the fluid-fluid spatial correlations between the fluid molecules and the external potential produced by the solid structure. These findings are supported by a comparison with experimental data and Grand Canonical Monte Carlo (GCMC) simulations of the adsorbed amount and density profiles of the adsorbed fluid inside the solid. One important parameter related to the accuracy involved in the DFT calculations is choosing the appropriate grid size. We proposed a priori grid size that is crucial in 3-D-DFT calculations. We also explore the impact of the non-crystalline structure of amorphous carbon nanopores on fluid structure and adsorption isotherms, as well as fluid-fluid and fluid-solid interactions. We offer insights for selecting computational methods in the fluid-structure analysis of nanoporous materials, guiding future research and optimization in advanced material development for diverse applications.

References:

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- 2) Elvis Soares, Amaro G. Barreto Jr., Frederico W. Tavares, "Classical Density Functional Theory Reveals Structural Information of H₂ and CH₄ Fluids Adsorption in MOF-5", *Fluid Phase Equilibria*, 574, 113887 (2023). DOI: 10.1016/j.fluid.2023. 113887
- 3) Lucas J. dos Santos, Elvis Soares, Amaro G. Barreto Jr., Frederico W. Tavares, "Comparison of 3D-cDFT and GCMC Simulations for Fluid-Structure Analysis in Amorphous Carbon Nanoporous Materials", *Adsorption*, (2024). Submitted.

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