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Predictions of Solvation Pressure in Mesopores Based on Saam-Cole Theory

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Adsorption-induced deformation has been found to manifest in numerous natural and engineering processes, e.g., drying of concrete, water-actuated movement of non-living plant tissues, swelling of coal and shale, etc. [1]. The driving force for the deformation is solvation pressure –the pressure that a fluid adsorbed in a nanopore exerts on the pore walls. Solvation pressure can be calculated from the derivative of the grand potential of the adsorbed fluid, which in its own turn can be derived from the adsorption isotherm [2,3].
Adsorption isotherms of mesoporous materials can be calculated via various thermodynamic approaches, two of them are Derjaguin-Broekhoff-de Boer (DBdB) [4] and Cole-Saam (CS) models [5]. These models are based on similar thermodynamic equations to describe phase transitions in nanopores, considering the influence of the pore wall in the form of solid-fluid interaction potential. However, they use different simplifying assumptions. CS theory, in contrast to DBdB, takes into account the curvature influence on the potential, giving more rigorous predictions for the adsorption isotherms.
In this work we derived analytical expressions for solvation pressures in cylindrical and spherical pores based on CS theory and used these expressions to perform calculations of solvation pressure corresponding to adsorption of N2 and Ar in silica pores. We compared our results with the calculations based on DBdB theory [3]. We showed, that while the predictions of CS and DBDB theory for isotherms for both geometries differ noticeably, the difference between the solvation pressure isotherms is less pronounced. This conclusion justifies application of either of the two macroscopic methods for predicting adsorption-induced deformation of mesoporous materials.

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