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Monte Carlo simulation of argon adsorption in 3DOm carbon pores with potential based on spheres with openings

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Three-dimensionally ordered mesoporous (3DOm) carbon is produced by negative templating of spherical silica nanoparticles [1]. The final product represents a periodic nanostructure with spherical pores interconnected by openings. These materials are promising for application in separation and purification processes as adsorbents, and for natural gas storage of methane in the form of hydrates [2]. However, the process of storing methane in the confined spaces and the influence of pore structure and morphology on hydrate formation are unclear. Moreover, it is not entirely transparent how the pore morphology affects the behavior of even simple fluids, such as nitrogen and argon, adsorbed in these pores.
For our simulations of argon adsorption in the model 3DOm structure, we employed the grand canonical ensemble Monte Carlo (GCMC) method. Initially, we applied the full spherical solid-fluid interaction potential [3]. Then, for more precise modeling, we transformed our structure by removing two, four and six windows and applying periodic boundary conditions. Such representation aided us to build isotherms, which describe the experimental isotherms more rigorously than a spherically symmetric potential or a sphere with one opening [4]. Therefore, the described model is valuable for interpretation of experimental data of argon adsorption and has a potential to serve as a kernel for pore size distribution calculations.

References

1. W. Fan et al. Hierarchical nanofabrication of microporous crystals with ordered mesoporosity, Nat. Mater., 2008, 7.12, p. 984–991
2. L. Borchardt et al. Illuminating solid gas storage in confined spaces –methane hydrate formation in porous model carbons. Phys. Chem. Chem. Phys., 2016, 18, 20607
3. D.W. Siderius, L. D. Gelb. Extension of the Steele 10-4-3 potential for adsorption calculations in cylindrical, spherical, and other pore geometries, J. Chem. Phys., 2011, 135.8, p. 084703
4. G. Y. Gor, C. J. Rasmussen, A. V. Neimark. Capillary condensation hysteresis in overlapping spherical pores: a Monte Carlo simulation study, Langmuir, 2012, 28.33, p. 12100–12107.

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