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Simulation of capillarity-driven flow dynamics of water in nanoporous silica (MCM-41)

Capillarity-driven flows in pores a few nanometers in diameter play an important role in many natural and technological processes, for example in clay swelling, frost heave, catalysis and transport across artificial nanostructures, bio-membranes and tissues [1]. Here we present molecular dynamics simulations modelling the capillary flow of water into silica nano-pores (MCM-41) of around 3 nm diameter pore size. By the usage of water-water [2], water-silica [3] and silica-silica [4] forcefield implementations we are able to simulate the spontaneous imbibition dynamics of water into the silica pores. The simulations confirm that the dynamics of the penetration depth of the fluid L into cylindrical pores after time t can be described by the Lucas-Washburn equation, $L = \sqrt{v_i}\sqrt{t}$. v_i is the so-called "imbibition speed" that depends on the ratio of the fluid parameters, the fluid/wall interaction, the radius of the pores and the hydrodynamic slip-boundary condition [5]. Further, the capillary flow induced strain in the host material resulting from the surface stress release (Bangham effect) and the acting Laplace pressures are investigated on a nanoscopic scale [6]. Of particular interest is the observed anisotropy in magnitude of strain in lateral and longitudinal pore direction which lacks theoretical description yet. Therefore, the simulations contribute valuable insights to the understanding of imbibition induced strains in materials. In combination with small angle and wide angle X-ray scattering (SAXS/WAXS) measurements of imbibition induced strain the simulation will lead to an overall better understanding of capillary-driven flows and its effects on the the host material [7].

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