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Computer simulations of capillarity-driven water flow in nanoporous silica

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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 oriented silica nano-pores (MCM-41) of around 3 nm diameter pore size. By providing implementations of water-water [2], water-silica [3] and silica-silica [4] forcefields we are able to simulate the spontaneous imbibition dynamics of water into the silica pores. In this work we show that during imbibition in longitudinal and radial pore direction anisotropic strains can be observed that can be classified as two distinct types of strain. At the start and the end of the imbibition process the observed strains are almost instantaneous while during the imbibition process there are continuous changes of strain that scale with the imbibition progress. Overall the results of the simulations should lead to better understanding of capillary-driven flows in nanoporous material and the corresponding imbibition-induced strains of the host material on a single-pore scale.

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