Modelling liquid flow through nanopores on the nanoscale

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Abstract

Liquid chromatography is one of the most important separation techniques and has proceeded mainly along empirical knowledge from the expansive collection of experimental data by using chromatographic methods, spectroscopic methods and technical innovations in column packing, particle technology and equipment design. However, a classic liquid chromatography column, is a cylinder densely packed with mesoporous silica particles whose surface has been mostly chemically modified. In this work, we investigated the physisorption of water to functionalized silica surfaces and hydrophilicity properties of surface by molecular dynamics simulations. We built on previously gathered knowledge on chromatography to establish a unified picture of stationary phase and solute mobility in liquid chromatography. In analogy to previous studies, we utilized a crystalline SBA-15 structure as starting point for our modeling approach. Furthermore, we investigate the effect of functionalization using different loadings with silanol group (Si-OH) and trimethylsilyl groups (O-SI-$(CH_3)_3$). With this strategy, we hope to understand the effect of functionalization of silica on the physisorption of water molecules at the nanometer scale.