# Filling Mechanisms and Capillary Condensation of Water in Nanopores

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## ABSTRACT

We will discuss, from a molecular standpoint, the filling and capillary condensation of water in nanopores in the range 1 - 5 nm diameter. Molecular dynamics simulations are employed to examine the effect of the hydrophilicity and the diameter of the pores on the mechanisms leading to condensation and hysteresis in the sorption isotherms of water. We found two possible mechanisms, characterized by either a homogeneous or a localized growth of the adsorbed layers, and consistent with recent HNMR experiments in silica pores. The predominance of one path or the other depends on a balance between pore size and water-affinity of the interface.