# SDS Surfactants in Cylindrical Alumina Nanopores

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We employ extensive all-atom molecular dynamics simulations to study aqueous sodium (SDS) surfactant spatial distribution and aggregate structure inside cylindrical alumina nanopores. First, we determine the effect of confinement in the nanopore by comparing the aggregate structure observed in our system to those observed in simulations on flat alumina substrates and those in bulk water. The results suggest that confinement, and in particular the partition of the counterions near the active sites on the surface, affects the structure of the aggregates. We then expand on these results, and we investigate the effects due to surfactant concentration and ion-specific effects on the aggregate structure and mobility of the various molecular entities considered. We discuss the results in the context of applications such as water desalination.