ALL-ATOM MOLECULAR DYNAMICS MODELLING OF SURFACTANTS IN SOLUTIONS

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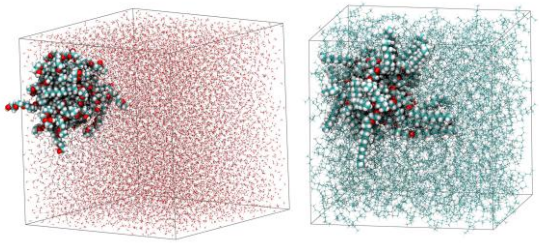
The results of all-atom molecular dynamics simulations of ionic and nonionic surfactants in polar and non-polar solvents are presented. Bulk systems that include direct or inverse micelles (see Figure) as well as surfactant monolayers at the water-hydrocarbon interface are simulated. Structural, transport, thermodynamic, and kinetic properties of the surfactant solutions are studied by analysing the molecular dynamics data.

The diffusion coefficients of direct and inverse micelles have been calculated using the Einstein formula [1]. The viscosities of micellar solutions have been estimated on the basis of the Stokes-Einstein relation [2]. The interfacial tension at the water-decane interface in the presence of different surfactants has been calculated on the basis of diagonal components of the pressure tensor [3]. The distribution of inverse micelles by their aggregation numbers is studied. The dependence of the obtained results on the simulation cell size is taken into account. MDynaMix and GROMACS software packages have been used to perform molecular dynamics simulations within CHARMM36 and CGenFF force fields. The simulation times range from several tens of nanoseconds to microseconds.



Direct and inverse micelles of $C_{12}E_4$ in water at T=298 K
and in heptane at T=223 K, correspondingly

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