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Structure and dynamics of water confined within reverse micelles

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— The structure and dynamics of water confined within reverse micelles (RMs) of varying water content ([water]/[surfactant]) formed by the surfactant Aerosol-OT in iso-octane are studied using molecular dynamics simulations. The intrinsic density profile of water in the RM is constructed with respect to the surface formed by the surfactant sulfur atoms and reveals a high density shell at the surfactant interface, a core region which becomes more bulk-like as RM size increases and an intermediate region between the interface and core. Water diffusion in the presence of partially absorbing boundaries (compatible with the intrinsic profile) provides a simple picture for describing confined diffusion within the RM. Water reorientation is strongly perturbed with respect to bulk water due to the presence of surfactant head groups and counterions. Our results for water dynamics in RMs are compared with the results of time-resolved IR and quasielastic neutron scattering experiments.

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