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MOLECULAR DYNAMICS STUDY OF WATER DYNAMICS AROUND THE SURFACTANT MONOLAYER ADSORBED AT THE AIR/WATER INTERFACE

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A constant volume and temperature (NVT) molecular dynamics (MD) simulation has been carried out to investigate the properties of a monolayer of monododecyl diethylene glycol ($C_{12}E_2$) surfactant adsorbed at the air/water interface at a surface coverage corresponding to that at its critical micelle concentration (34 $Å^2$/molecule). The study shows that the surfactant monolayer strongly influences the translational and rotational mobility of interfacial water molecules. A drastic change in the dipolar reorientational motion of water molecules in the aqueous layer is observed with a small variation of distance from the surfactant headgroups.

Keywords: ***Molecular Dynamics, NVT, Monolayer***