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Molecular fragment dynamics study on the water-air interface behavior of non-ionic polyoxyethylene alkyl ether surfactants

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Molecular Fragment Dynamics (MFD) is a mesoscopic simulation technique based on Dissipative Particle Dynamics (DPD). Whereas DPD beads in general may not necessarily be identified with chemical compounds at all the MFD variant uses specific molecules or molecular fragments as its basic *coarse-grained* interacting entities (rather than the *fine-grained* atom types of Molecular Mechanics). MFD can be used to study formulations of drugs and active agents in oil, water and emulsions.

MFD simulations of the nonionic polyoxyethylene alkyl ether surfactants C_6E_6, $C_{10}E_6$, $C_{12}E_6$ and $C_{16}E_6$ at the water-air interface are performed to study their nanoscale structures and surface properties. The simulations of the self-aggregation of the polyoxyethylene alkyl ether surfactants lead to equilibrium nanoscale structures and computationally determined surface tensions which are in agreement with experimental data for different surfactant concentrations [1].

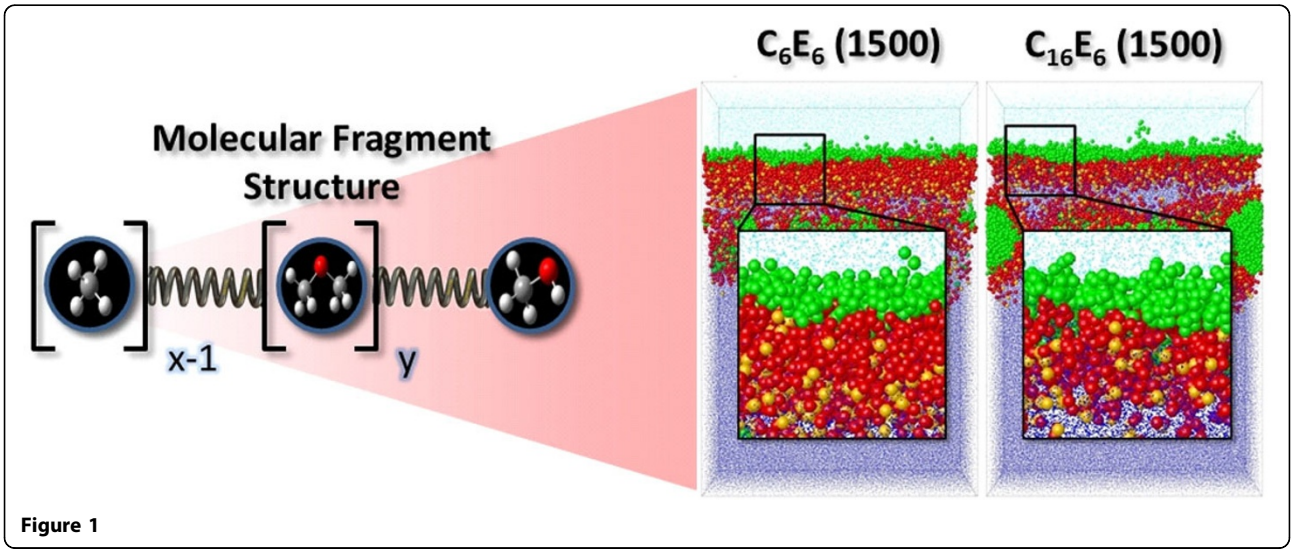

Figure 1

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