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

Andreas Truszkowski[1*], Annamaria Fiethen[2], Hubert Kuhn[2], Thomas Wiebringhaus[3], Achim Zielesny[3], Matthias Epple[1]

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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].

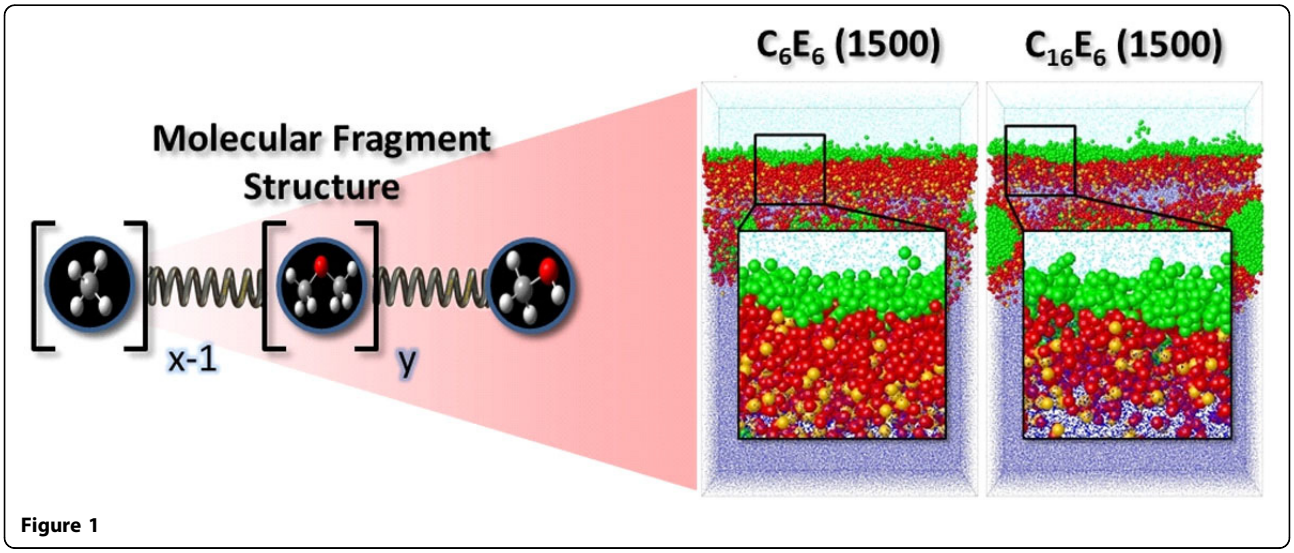


**Figure 1**

[1]Inorganic Chemistry and Center for Nanointegration, University of Duisburg-Essen, Essen, 45141, Germany
Full list of author information is available at the end of the article

**Authors' details**
[1]Inorganic Chemistry and Center for Nanointegration, University of Duisburg-Essen, Essen, 45141, Germany. [2]CAM-D Technologies, Essen, 45117, Germany. [3]Institute for Bioinformatics and Chemoinformatics, Westphalian University of Applied Sciences, Recklinghausen, 45665, Germany.

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