Complex nanostructured self-assemblies such as colloidal suspensions, micelles, immiscible mixtures, microemulsions, etc., represent a challenge for conventional methods of simulation due to the presence of different time scales in their dynamics. In this work the novel computer simulations technique, Dissipative Particle Dynamics (DPD) has been applied to model the self-aggregation of amphiphiles in aqueous systems, microemulsions and at the water-air interface. The DPD parameters have been calculated by Monte-Carlo Simulations and this work showed that the parameter calculation used is suitable for complicated systems. The application of Dissipative Particle Dynamics studies of amphiphilic surfactants in aqueous solution has been successfully extended to the complicated poly (ethylene oxide) - *block*- poly (propylene oxide) -*block*- poly (ethylene oxide) triblock copolymers. The computationally achieved phase diagram of $EO_{13}PO_{30}EO_{13}$ in water at 300K was in remarkable agreement with the experimental phase diagram and showed the micellar, hexagonal, lamellar and inverse micellar phase.

The less complicated surfactants $C_{10}E_4$, $C_{12}E_5$ and $C_{12}E_6$ have been investigated with DPD to yield structural data of the observed phases. I have successfully applied Dissipative Particles Dynamics to simulate the self-assembly of $C_{10}E_4$ and $C_{12}E_5$ in water. It was possible to distinguish between the isotropic L_1 and L_2 phases as well as the lamellar L_α phase. The simulated bilayer thickness of $C_{10}E_4$ was ε_{sim}=4.9nm which is in good agreement with the experimental value of ε_{exp}=5.0nm±0.5nm. The micellar aggregation number for $C_{10}E_4$ was calculated to 53±10 molecules. The bilayer thickness and aggregation number for $C_{12}E_5$ and $C_{12}E_6$ were calculated as well. $C_{12}E_5$ gave a simulated bilayer thickness of ε_{sim}=6.3nm in comparison to an experimental value of ε_{exp}=6.0nm and a micellar aggregation number of 98±14. The simulated bilayer thickness of $C_{12}E_6$ was ε_{sim}=7.7nm and the simulated micellar aggregation number was 79±16 which is very close to the experimental value of 87. This structural investigation proved that the DPD method is not just suitable to reproduce the phase behavior of amphiphilic surfactants and polymers qualitatively but also quantitatively.

The DPD simulation of microemulsion systems has not been compared in the literature with experimental results but was applied on model surfactants. The Dissipative Particles Dynamics method to simulate the self-assembly of $C_{10}E_4$ in water has been successfully used. It was possible to distinguish between the w/o, o/w and bicontinuous microemulsions as well as the lamellar L_α. The simulation results of $C_{10}E_4$ in water and n-decane are in good agreement with the experimental phase diagram.

The X-point shift has been found at a concentration very close the experimental value. The simulation of the quaternary system $C_{10}E_4$/PEP5-PEO5/water/n-decande did also match the experimental results very well and the boosting-effect was found computationally with DPD. The possibility to easily modify the polymer as well as the surfactant to observe the influence of these changes to the so-called X-point opens up a great opportunity to many industrial applications. The X-point characterizes the efficiency of a surfactant in washing processes. The simulation results of the X-point shift from γ=15% (δ=0%) to γ=10% (δ=5%) are in remarkable agreement with the experimental values. The boosting–effect could not be observed by adding a PPO5-PEO5 diblock copolymer which agrees with the experimental results where these systems also did not show an X-point shift.

It was now possible to get a detailed insight into the mechanism of the boosting–effect with this novel computer simulation technique. Experiments suggested that the mechanism of the boosting-effect is more likely based on the modification of the structure of the bicontinuous microemulsion phase by smoothing the interface caused by the polymer. The replacement of surfactant molecules by the bigger polymer molecules which would not depend significantly on the kind of polymer is not important. The computer simulations support the assumption that the change of the bicontinuous microemulsion structure caused by the polymer molecules play the major role in the mechanism and that the replacement of surfactant molecules by the polymer is not as important.

It was also possible to calculate the experimentally unknown phase behavior of poly (ethylene butylene)-*block*-poly (ethylene oxide) diblock copolymer in water and methyl cyclohexane. The three different phases found like oil-in-water, water-in-oil droplets and a bicontinuous microemulsion phase, as well as the character of the thermodynamic model, indicate the formation of a microemulsion in this polymer/water/oil system. The DPD method has been applied to an experimentally uninvestigated system for the first time and produced interesting results. With these new insights in the phase behavior of the polymer – water – oil system many new applications are possible.

The introduction of the air beads into the DPD methods opens up a wide range of new applications. For the first time the surface tension has been calculated with Dissipative Particle Dynamics while the systems published in the literature just dealt with interfacial tension between two condensed phases. The shape of the experimental surface tension diagram of $C_{10}E_4$, $C_{12}E_5$ and $C_{12}E_6$ at the water – air interface has been reproduced with DPD. In the simulated as well as in the experimental graphs $C_{10}E_4$ has a clearly higher *cmc* with a lower surface tension than $C_{12}E_5$ and $C_{12}E_6$ which have very similar *cmc* and surface tension. The conversion of the DPD surface tension to physical units shows an acceptable agreement. Together with the qualitative agreement of experiments and simulations the quantitative comparison makes predictions of surface tension of unknown surfactants and polymers possible.

All calculation results are in remarkable agreement with the experimental data. In the present work the applications of the method have been extended significantly. The simulation of simple surfactant-water systems has been used to obtain structural information. Oil has been added and even microemulsion formations of ternary and quaternary systems have been observed. A completely new field – the DPD calculation of the surface tension – has been opened by the introduction of air beads.

The DPD method proved to be a reliable tool to get a better understanding of the nanostructure of self-assemblies and structural information. It was even possible to investigate an experimentally unknown system and the method is therefore applicable to support the often complicated experiments or even to obtain experimentally unavailable data. With this method it is easily possible to predict the properties of compounds and in this way to avoid expensive experiments by suggesting promising candidates for certain industrial applications. To our knowledge DPD is a unique method to simulate mesoscopic structures on a relatively long time scale based on an intermolecular interaction level.