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MFD-simulation of surface coatings – an extension to solid/fluid molecular modelling models

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Molecular Fragment Dynamics (MFD) is a new method for mesoscopic molecular modelling computer simulations derived from Dissipative Particle Dynamics (DPD) [1]. It can be used to simulate dynamical processes at a microsecond timescale and up to micrometer scales and can handle up to 1.500.000 particles. This unique technique so far has been successfully applied to surfactants, adjuvants, polymers, nanoparticles and complex mixtures thereof in materials and life science simulation studies [2].

MFD has been applied to a system of different glyceroldialkylnomizoltetraetherlipid (GDNT) concentrations at different solvent / solid borofloate substrate interfaces. GDNT is a tetraetherlipid won from archaebacteria and known for its antifouling capabilities. This scheme was applied in order to find out at which concentration and in which solvent the best levels of GDNT aggregation could be reached and how such coated glass surfaces look like.

A brief introduction to the MFD theory and the procedure will be given. From the simulation results the aggregation of GDNT at the solvent / borofloat interface can be shown. The influence of the different solvents and concentrations on the aggregation process is discussed in detail. The simulations reveal differences of the molecular conformations of the GDNT at the interface and the effect demonstrated on a molecular level. By considering these calculations we show the transfer of real surface structures to a molecular model used in MFD simulations.

References

1. Jensen F: *Introduction to Computational Chemistry John Wiley & Sons, New York*; 2006.
2. Richter DS, *et al.*: *Proceedings for the ISAA 207 (on CD)* 2007.