Simulations of amphiphilic worms, bi-layers and vesicles in equilibrium and in shear flow

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Depending on molecular structure and on thermodynamic conditions amphiphilic molecules may self-assemble in a great variety of structures, of which we will discuss bi-layers, worms and vesicles.

The free energy of bi-layers in general contains contributions from stretching and bending the bi-layer and from its edges. We will present the results of calculations of all these contributions. In particular we will discuss the role of the edge free energy in determining the phase diagram of punctured bi-layers. Driven by the minimization of the edge free energy freely floating discs will curve into cups and finally close to form vesicles. Examples of simulations of this process will be given.

We will discuss results of simulations of bi-layers in shear flow with the shear-gradient perpendicular to the bi-layer. From these simulations we extract the friction forces that occur when the two layers of the bi-layer slide along each other. At extremely large shear rates the bi-layer ruptures and forms cylinders.

At the end of the presentation we discuss bending and buckling of amphiphilic worms and the contribution of the end-caps to their free energies. Finally we discuss some elementary processes occurring at entangled worms and their relevance for the extreme shear thinning of worm like micelles.