

# Transferability problems of coarse grained models for systems with soft interfaces

Christine Peter

*University of Konstanz, Germany*

One of the major challenges for multiscale simulations is the representation of conformational transitions when macromolecules interact with membranes or interfaces. For example, soft interfaces interfere with the conformational equilibrium of proteins between intrinsically disordered states, beta-sheets or alpha helices, causing major shifts in that equilibrium which can be linked to function/malfunction of these proteins. Reproducing the correct conformational response of a biomacromolecule is extremely important for multiscale simulations, and a particular challenge for coarse grained models. I will present a few examples of such effects which are designed to investigate the general physical principles that contribute to environment-induced conformational transitions and that show how they can be approached in coarse grained modelling.

[1] C. Dalgicdir, O. Sensoy, C. Peter and M. Sayar, *J. Chem. Phys.* 139 234115 (2013) [2] C. Dalgicdir, C. Globisch, M. Sayar and C. Peter, *Eur Phys J Spec Top.* 225 1463–1481 (2016)