171st MSS Seminar
Wednesday, October 4, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Institute for Multiscale Simulation
MSS

Free energy analysis of the molecular transport into amphiphilic self-assembly systems

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Self-assemblies of amphiphilic molecules, such as lipid membranes and micelles, can flexibly change their local structures while maintaining their whole shape. This property enables them to take up and transport materials. Understanding intermolecular interactions, including solvents and ions, is essential to finding ways to control the distribution and transport of substances. In this talk, I will show the free-energy analysis of the binding and transport of a molecule in micelle and bilayer membrane by molecular dynamics simulations. In the micelle system, we control the diffusion of surfactant molecules to make a sharp boundary. By calculating the free-energy profile in transporting of a hydrophobic molecule into the micelle, we investigate the effect of boundary roughness on the transport property. The results reveal that a sharp boundary induces the free energy barrier at the interface and the stableness of a molecule in the center of micelle. In the membrane system, we examine the stabilities of a variety of binding configurations of a small peptide in two kinds of bilayers. The binding free energy is calculated, and it is seen that the transmembrane configuration is stable in both membranes. A surface-bound state is also found to be stable due to the balance between the attractive and repulsive interactions of the peptide with lipid and water.