

MD Simulation of Micelle Formation

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The goal of the hands-on module "Molecular Dynamics Simulation of Micelle Formation" is to make the students acquainted with some necessary knowledge about how to plan, set up and run a molecular dynamics simulation of a system of disordered molecules. Since neither completely random nor completely ordered arrangements of molecules form the best starting point, special tools need to be used to efficiently generate suitable starting configurations for such simulations. We will explain the use of the frequently used tool 'moltemplate' [<http://moltemplate.org>], which allows the creation of regular arrays and random systems of various templated molecules. Solvation of such molecular systems with a solvent (here: water) will be achieved by the use of the tool 'packmol' [<http://www.ime.unicamp.br/~martinez/packmol/home.shtml>], which allows starting from a dense systems with few bad molecular contacts, so that efficient and fast equilibration is possible. Simulations are performed with the versatile classical MD engine 'lammmps' [<http://lammmps.sandia.org>]. The progress of system equilibration and some data analysis strategies will be discussed using the visual MD program 'vmd' [<http://www.ks.uiuc.edu/Research/vmd>] and specific tools developed in our own group.