



"Soft-Matter Seminar"

Dr. Alexander Lyubartsev

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Title: Multiscale modeling of lipid bilayers

A multiscale modeling approach is applied for simulations of lipids and lipid assemblies on mesoscale. First, molecular dynamics simulation of initially disordered system of lipid molecules in water within all-atomic model was carried out. On the next stage, structural data obtained from the molecular dynamics (MD) simulation were used to build a coarse-grained (ten sites) lipid model, with effective interaction potentials computed by the inverse Monte Carlo method. Finally, several simulations of the coarse-grained model on longer length- and time-scale were performed, both within Monte Carlo and molecular dynamics simulations: a periodical sample of lipid molecules ordered in bilayer, a free sheet of such bilayer without periodic boundary conditions, formation of vesicle from a plain membrane, process of self-assembly of lipids randomly dispersed in volume. We show that the coarse-grained model, developed exclusively from all-atomic simulation data, reproduces well all the basic features of lipids in water solution.

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16:00 Uhr

Raum PH 3344

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