Physikalisches Institut

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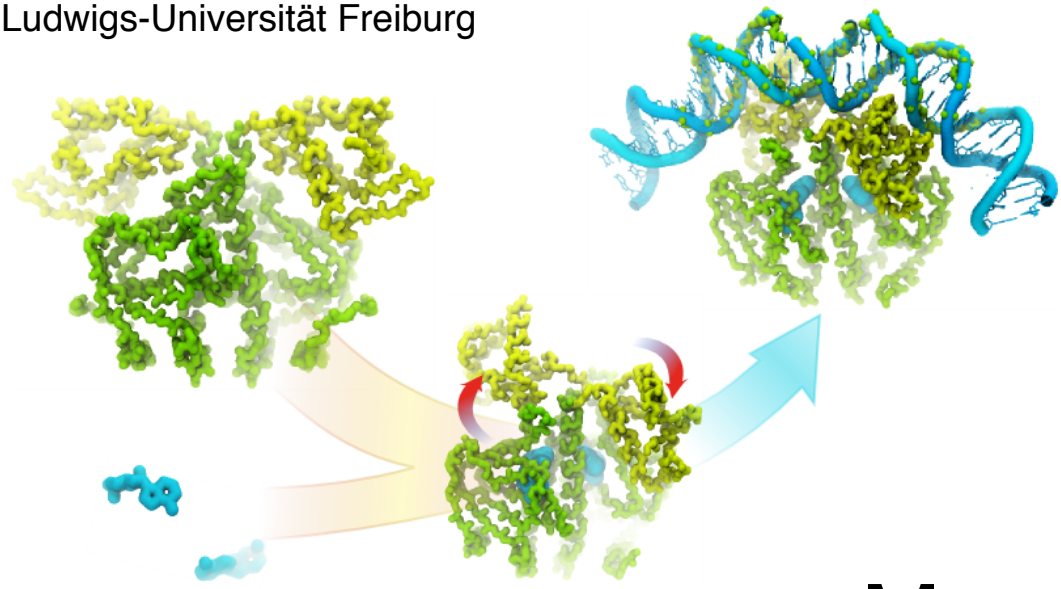

May 16

Membrane molecular dynamics force fields

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The all-atom optimized potentials for liquid simulations (OPLS-AA) force field is a popular force field for simulating biomolecules. Here, we optimized the OPLS-AA force field for both short and long hydrocarbons, as well as for phospholipids. Following the framework of the OPLS-AA parametrization, we refined the torsional parameters for hydrocarbons by fitting to the gas-phase ab initio energy profiles calculated at the accurate MP2/aug-cc-pVTZ theory level. Additionally, the Lennard-Jones potential was adjusted to reproduce the densities and the heats of vaporization of alkanes and alkenes of different lengths. Optimization of partial charges finally allowed to reproduce the gel-to-liquid-phase transition temperature for pentadecane. It is shown that the optimized parameter set (L-OPLS) yields improved hydrocarbon diffusion coefficients, viscosities, and gauche-trans ratios. In a second step, L-OPLS was extended to cover frequent phospholipids. Its applicability for lipid bilayer simulations is shown for various phospholipid bilayers.

Molecular Dynamics Seminars 2012

Seminar Room of Gustav Mie Haus, Ground Floor, 16:15

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