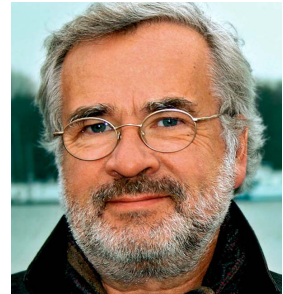# IAP Seminar

Michael Grunze

Max-Planck-Institut für medizinische Forschung,
Department of Cellular Biophysics
Heidelberg/Germany

Tuesday, 23th January 2018, 16:00 s.t.
TU Wien, Institut für Angewandte Physik, E134
1040 Wien, Wiedner Hauptstraße 8-10
Yellow Tower „B", 5th floor, SEM.R. DB gelb 05 B

Computer Simulation Of Water-Mediated Adhesion Between Organic Surfaces: Dissecting The Forces

The adhesive forces operating between various surfaces in aqueous media are of interest in many areas ranging from biology to electronics. This refers, in particular, to supported lipid membranes where the water-mediated bilayer-substrate adhesion determines the stability of the system, and surfaces formed by self-assembled monolayers (SAMs) on solid substrates to modify the surface-sensitive properties of the latter.

We used the grand canonical Monte Carlo technique to reveal the origin of the repulsive pressure operating between supported DLPC bilayers at short separations. By partitioning the inter-bilayer pressure into physically distinct components, it is shown that the short-range repulsion comes mainly from the direct electrostatic lipid-lipid interaction of the head groups in the opposing leaflets. By contrast, the electrostatic lipid-lipid interaction between DLPE bilayers is strongly attractive, and the short-range repulsion is associated with the hydration (water-lipid) interactions. These simulations explain why DLPC bilayers have a much larger inter-bilayer (fluid) separation at a given pressure, as compared to that for DLPE.

We extended the models to model the interactions between a hydrophobic methyl-terminated SAM (C-SAM) and an hydrophilic carboxyl-terminated SAM (hereafter, O-SAM), with phosphatidylethanolamine (PE) bilayers. The free energies of adhesion were evaluated by integration of simulated pressure-distance relations. For SAMs, both symmetric and asymmetric confinements were considered, as formed by like and unlike SAMs, respectively. The total values of the free energies of adhesion are in acceptable agreement with available experimental data. The analysis of the partial energies in the total free energies of adhesion provide a mechanistic model of "hydrophobic" and "hydrophilic" interactions in water.

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion)

Friedrich Aumayr
(LVA-Leiter)

Ulrike Diebold
(Seminar Chair)