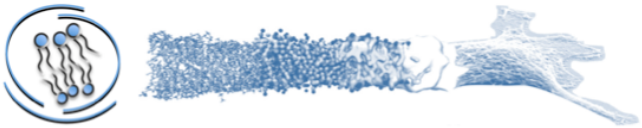
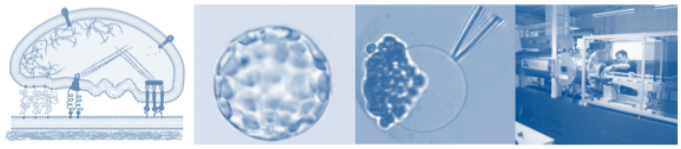

Research Training Group 1962

Dynamic Interactions at Biological Membranes from Single Molecules to Tissue

Speaker: Prof. Dr. Rainer Böckmann, Computational Biology

Invitation to RTG 1962 – Guest Talk

Tuesday, 22nd October 2019 at 17.00 (s.t.)

Prof. Dr. Andreas Heuer

(University of Münster)

"Formation of membrane domains: insight from simulations on different coarse-graining levels"

The understanding of domain formation in lipid membranes is challenging due to the large time and length scales involved in this process. In my talk I will be present different simulation approaches to approach this problem.

(1) Via very long simulations on the atomistic scale we managed to see the onset of raft formation in ternary lipid mixtures.
(2) Many orders of magnitude more efficient are simulations on a coarse-grained level, using the Martini force field. Indeed, in turns out that the raft formation, analysed on the atomistic or the coarse-grained level, behave very similarly.
(3) Recently, we managed to map a lipid membrane on a lattice model. All parameters of that model can be extracted from short molecular dynamics simulations. It is shown, e.g., for a pure DPPC membrane, that the Monte Carlo simulation of the corresponding lattice model reproduces, e.g., the transition between the gel-phase and the liquid disordered phase.

Finally, the special properties of sterol molecules (cholesterol and ergosterol) as compared to phospholipids as well as the impact of transmembrane domains on the lipid structure are discussed.

Guests are welcome!

gez. Prof. Dr. R. Böckmann

→ *Venue: Department Biology, Seminar Room Cell Biology (00.581), Building B1, Floor 00, Staudtstraße 5, 91058 Erlangen*