

Seminar

"IRTG: Soft Matter Science "

### Modulating the Structure and Properties of Cell Membranes by Small Amphiphilic Molecules: Insight form Computer Modeling

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Recipient of the Bessel Research Award of the Alexander von Humboldt-Foundation

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## Wednesday, February 2, 14h15

"Hörsaal Makromolekulare Chemie", Stefan-Meier-Str. 31, Freiburg

You are welcome to meet Dr. Andrey Gurtovenko after the seminar. Do not hesitate to contact Christelle Vergnat (<u>softmattergraduate@physik.uni-freiburg.de</u>) to organize a meeting.









### Dr. Andrey Gurtovenko

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#### Modulating the Structure and Properties of Cell Membranes by Small Amphiphilic Molecules: Insight form Computer Modeling

Manipulating the structure and properties of cell membranes is an issue which is fundamental to numerous applications in the biosciences, pharmaceuticals, and biotechnology. To induce formation of transient structural defects in membranes, various factors such as external electric and mechanical forces, surfactants, antimicrobial peptides, and polyelectrolytes could be applied to the membrane. Here we employ atomic-scale molecular dynamics simulations to reveal a molecular level picture of how small amphiphilic molecules affect the structural and mechanical properties of phospholipid membranes. We demonstrate that specific modes of action of such molecules depend on both chemical structure and concentration of amphiphilic molecules. In particular, in a certain concentration range one can witness formation of water pores and micelle-like structural defects in lipid bilayers, a phenomenon which is highly relevant to trafficking across cell membranes.

A. A. Gurtovenko, J. Anwar, I. Vattulainen, *Chemical Reviews* **110**, 6077-6103 (2010).