KEMIJSKI INŠTITUT

Vabilo na predavanje / Invitation to the lecture

Sreda / Wednesday, 5.4.2023 ob / at 11:00
Velika predavalnica Kemijskega inštituta / Great Lecture Hall

Prof. dr. An Ghysels

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Predicting the permeability of phospholipid membranes with molecular dynamics simulations

Permeability is a key property of biological membranes. Several strategies have emerged to predict membrane permeability from molecular dynamics (MD) simulations, which suffers from slow convergence of the statistics. The counting method, the Bayesian analysis to an inhomogeneous diffusion model, and a new methodology based on path sampling are presented. These methodologies are challenged in various applications. As a first application, oxygen transport is discussed, where oxygen should cross the membrane to reach its final destination at the cytochrome c oxidase protein where it is consumed. Next, the transport in so-called rafts is investigated, which are ordered regions floating in the generally disordered two-dimensional sea of phospholipid molecules. For some applications, the methodologies needed to be made compatible with curved membranes instead of flat membranes. An example of curved membranes is the residence time of drug molecules captured inside liposomes, which are small spherical membrane particles used as nanocarriers for e.g. vaccines. Another example of curvature is transport through caveolae, which are highly curved membrane invaginations that are characteristic for young healthy heart cells, but which gradually flatten with age for unknown reasons. Finally, the oxygen transport in grey matter is discussed, since axons in the brain are surrounded by myelin sheets consisting of stacked membranes.[1,2]

[1] A. Ghysels, A. Krämer, R. M. Venable, W. E. Teague Jr, E. Lyman, K. Gawrisch, R. W. Pastor, Nature Communications 10 (2019) 5616

[2] S. Davoudi, A. Ghysels, Biophysical Journal (2022) doi: 10.1016/j.bpj.2022.11.028

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