Free energy of lipid membrane pores in electric field

Gari E. Kasparyan and Jochen S. Hub

Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Lipid membranes define biological cells by establishing a semi-permeable barrier. Pore formation plays a role in processes such as membrane fusion and fission, the killing of bacterial cells with antimicrobial peptides, and others. Experiments have provided hints to the free energy of pore formation almost 40 years ago. Although pores are heavily studied with a variety of methods, the free energy profile of the initial stages of the pore formation is still not fully understood. We use molecular dynamics simulations to study the mechanisms and energetics of pore formation. The challenge of exploring the free energy landscape is overcome with Umbrella Sampling along a new reaction coordinate [1]. Electric fields have been used in electroporation to facilitate formation of pores for uptake of genes and drugs. The current work builds on results for tension-free membranes [2] by studying the effects of different electric fields. Our preliminary results show a significant drop in the free energy of the open pore upon introduction of electric fields.

[1] J. S. Hub and N. Awasthi, *J. Chem. Theory Comput.* 2017, *13, 2352−2366*
[2] C. L. Ting, N. Awasthi, M. Müller, and J. S. Hub, Phys. Rev. Lett., 2018, 120, 128103