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Nucleation Barriers in Lipid Membranes - From Thermotropic Phase Transitions to Membrane-Catalyzed Cavitation

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Lipid-based bilayer membranes are major components of all life forms and often subject to various temperature and pressure conditions. By combining atomistic molecular dynamics simulations with kinetic modelling, we have investigated the thermotropic chain melting phase transition in lipid bilayers [1] and the formation of cavities inside lipid bilayers [2]. The latter can occur when the cohesion of biological liquids is challenged by volumetric tension (i.e., "negative pressure"), which typically applies to the sap in plant conduits. We found that cavity formation in lipid bilayers under certain conditions can catalyze catastrophic embolisms in plants but under other conditions is also suited to prevent intolerable tensions in the sap.

[1] B. Kowalik, T. Schubert, H. Wada, M. Tanaka, R.R. Netz, E. Schneck, J. Phys. Chem. B, 119, 14157 (2015)

[2] M. Kanduc, E. Schneck, P. Loche, S. Jansen, H.-J. Schenk, R.R. Netz, Proc. Natl. Acad. Sci. USA, 117, 10733 (2020)