342d Stabilization of Model Membrane Systems by Disaccharides. Quasielastic Neutron Scattering Experiments and Atomistic Simulations

Emmanouil Doxastakis, Victoria Garcia Sakai, Satoshi Ohtake, Janna K. Maranas, and Juan J. de Pablo

Trehalose, a disaccharide of glucose, is often used for the stabilization of cell membranes in the absence of water. This work studies the effects of trehalose on the structure and dynamics of model membrane systems as they undergo a melting transition using a combination of experimental methods and atomistic molecular simulations. Quasielastic neutron scattering experiments on selectively deuterated samples provide the incoherent dynamic structure over a wide time range through the use of both time-of-flight and backscattering spectrometers. Elastic scans probing the lipid tail dynamics display clear evidence of a main melting transition that is significantly lowered in the presence of trehalose. Lipid headgroup mobility is considerably restricted at high temperatures and directly associated with the dynamics of the sugar in the mixture. Molecular simulations are employed to explore the nature of the motions present in the samples prior to and after the main transition. Changes in thermodynamic properties such as the area per lipid and the orientation of the chains are calculated at different temperatures. A detailed overview of the dynamics and their spatial and time dependence is also provided. The combined simulation and experimental methodology employed in this work offers a unique, molecular view of the physics of systems commonly employed in cryopreservation and lyophilization processes.