

139e Molecular Simulations of Multicomponent Bilayers. the Effect of Disaccharides, Cholesterol and Lipid Composition on Membrane Properties

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Atomistic molecular dynamics simulations are used to provide insights into the changes induced by the role of trehalose in hydrated lipid bilayer systems containing significant amounts of cholesterol, a component found in large quantities in cell membranes of cells. Trehalose, a disaccharide of glucose, is often used for lyophilization of cells. This sugar is found to display important stabilizing properties even in the presence of sterols and competes with the reported condensing ability of cholesterol. The dynamics of the systems are considerably modified by the partitioning of different components in the hydrophilic and hydrophobic regime of the membrane, with the whole lipid motion being restricted to a large extent by either trehalose or cholesterol. On larger spatial scales, lipid mixtures are studied by concurrent use of appropriate coarse grained models, and a novel Monte Carlo methodology that relies on extended configurational sampling and order-parameter sampling of the systems of interest. Changes in head group chemical structure and chain length induce an apparent modification of the mechanical properties of lipid bilayers. The employed Monte Carlo technique provides an efficient approach to study the composition dependent properties of multicomponent membrane models.