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Molecular simulation studies of edges in bilayers and bicelles[1]

JAMES KINDT, Emory University, Department of Chemistry

The instability of the free edge of a lipid bilayer can be quantified by a line tension, or excess free energy per unit length of the edge. Atomistic simulations of bilayer ribbons composed of a series of lipids with varying tail lengths and degrees of saturation have been performed to determine line tensions, with the goal of relating edge stability to structural and elastic properties of the bilayer. Line tensions are relevant to the mechanical stability of bilayer membranes, and can be reduced or eliminated by the inclusion of edge-stabilizing molecules (edge-actants) to the bilayer system. Mixtures of long- and short-tailed phospholipids are known to form aggregates known as "bicelles" that contain bilayers with stable edges. Simulations of "bicelle" mixtures using coarse-grained and atomistic lipid models have been performed to study the partitioning of short-tailed lipids towards the edge and the flexibility of the stabilized edge. Input from these simulations has been used in the development of simple thermodynamic models to rationalize some aspects of bicelle aggregate morphology.

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