The Molecular Structure of the Liquid Ordered Phase

EDWARD LYMAN, University of Delaware — Molecular dynamics simulations reveal substructures within the liquid-ordered phase of lipid bilayers. These substructures, identified in a 10 μsec all-atom trajectory of liquid-ordered/liquid-disordered coexistence (L₀/Lₐ), are composed of saturated hydrocarbon chains packed with local hexagonal order, and separated by interstitial regions enriched in cholesterol and unsaturated chains. Lipid hydrocarbon chain order parameters calculated from the L₀ phase are in excellent agreement with ²H NMR measurements; the local hexagonal packing is also consistent with ¹H-MAS NMR spectra of the L₀ phase, NMR diffusion experiments, and small angle X-ray- and neutron scattering. The balance of cholesterol-rich to local hexagonal order is proposed to control the partitioning of membrane components into the L₀ regions. The latter have been frequently associated with formation of so-called rafts, platforms in the plasma membranes of cells that facilitate interaction between components of signaling pathways.

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