Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

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 (L_o/L_d), 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 L_o phase are in excellent agreement with ^{2}H NMR measurements; the local hexagonal packing is also consistent with ^{1}H-MAS NMR spectra of the L_o 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 L_o 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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Date submitted: 14 Nov 2013 Electronic form version 1.4