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Phase Behavioral and Structural Properties of an Efficient Solvent-Free Model of Lipid Bilayers[1] JOEL REVALEE, MOHAMED LARADJI, University of Memphis — High-power computers facilitate the study of lipid bilayer membranes. Any computer model used to simulate such membranes must account for their spontaneous self- assembly due to hydrophobic interactions between lipid tails and water. This is usually done by simulating lipid molecules in explicit solvent. In such simulations most of the system is occupied by the solvent. It is therefore computationally desirable for equilibrium studies of lipid membranes to develop a model that leads to self-assembly of lipids without explicit solvent. We designed such a model, and show that its use leads to faster simulations than what can be achieved with current solvent-free models. This model utilizes soft interactions to account for hydrophobic effects (instead of the Lennard-Jones potential). Investigation of the lipids' diffusion coefficient, single-lipid orientational order parameter and internal energy as functions of temperature reveal a structural phase diagram in the membrane from a gel-like hexatic phase to a fluid phase. The characterization of membrane elastic properties from this model will also be presented.

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