393d Structure and Dynamics of Lipid Membranes: How Can Simulations Aid Experiments?

Jeffery B. Klauda, Bernard R. Brooks, and Richard W. Pastor

Molecular dynamics (MD) can be used to better understand the three-dimensional structure and dynamics of the biologically relevant liquid crystalline (L_α) phase. We present ten nanosecond simulations of a dimyristoyl phosphatidylcholine (DMPC) bilayer with five surface areas per lipid (A) (55.0, 59.7, 60.7, 61.7, and 65.0 $Å^2$) and the CHARMM27r (C27r) force field to gain insight into the component structure and A for DMPC (A^{exp}=60.6 $Å^2$). Experimentally the distribution of lipid components is obtained from structural models (SM) fit to the data. A new SM is developed that includes kurtosis of the methyl distribution with insight from our MD simulations. Moreover, the fundamental parameter A is refined with the new SM model. Together this approach resolves the experimental-simulation discrepancy for the methyl trough and A.

While lateral motion of lipids is straightforward to determine from experiments, it is difficult to resolve rotational and internal motions and thereby to determine values for components of the rotational diffusion tensor. Recent, ^{31}P NMR measurements have suggested that the relaxation of the phosphorous-carbonyl hydrogen vector is dominated by axial diffusion on the 5-10ns time scale, depending on the lipid. Results of three 50 ns simulations of dipalmitoyol phosphatidylcholine (DPPC) and analysis of correlation functions and first passage times yield $D_{\|} \approx 1 \times 10^8\ s^{-1}$ and thereby support the experimental proposal.