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Efficient calculation of mechanical properties of multicomponent phospholipid bilayers with Monte Carlo simulations MANAN CHOPRA, EMMANOUIL DOXASTAKIS , NICHOLAS L. ABBOTT, JUAN J. DE PABLO, UW Madison — We present a systematic study of the mechanical properties of multicomponent phospholipid bilayers. Two sets of systems are considered. The first consists of a mixture of DioleoylPhosphatidylethanolamine (DOPE) and DioleoylPhosphatidylcholine (DOPC) phospholipids. These two molecules have different head groups but the same chain length. The second system consists of a mixture of DilauroylPhosphatidylcholine (DLPC) and DistearoylPhosphatidylcholine (DSPC); these molecules have different chain lengths but the same head group. We use atomistic and coarse grain models, coupled to advanced Monte Carlo simulation techniques, to examine the structure and mechanical properties of the bilayers. Our results for pure systems are in quantitative agreement with experiment. Experimental data for mixed bilayers are not available, but our results indicate that their mechanical behavior is highly non-linear, a finding that we can interpret in terms of the composition and the resulting structure of the mixtures.

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