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Molecular Dynamics Simulation of the Fully Hydrated Dipalmitoylphosphatidylcholine (DPPC) Bilayer at Different Temperatures and Pressures[1] JOLANTA B. LAGOWSKI, Memorial University of Newfoundland, SURANJITH N. WANASUNDARA, University of British Columbia — The structural properties of lipid bilayers in biological membranes are of great interest in biochemistry, biophysics, and medicine. The main goal of this study is to use molecular dynamic (MD) techniques to investigate physical properties of the hydrated dipalmitoylphosphatidylcholine (DPPC) bilayer. The bilayer model consists of 25 DPPC molecules per each monolayer and 44.8% water by total weight. A modified version of AMBER MD suit of programs with CHARMM22 force field for phospholipids and the isothermal-isobaric or NPT ensemble with a fully flexible simulation box in ROAR program was used in this study. Simulations were performed under different pressure and temperature conditions. A liquid crystal phase (L_α) is (experimentally) expected with the DPPC bilayer under 1 atm pressure and 323 K temperature conditions. However, area per lipid, bilayer thickness, chain tilt, and the order parameters resulting from the present simulation appeared to be more consistent with the known properties of the $L_{\beta'}$ phase. The results of the simulations will be discussed.

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