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Cholesterol Flip-Flop Dynamics in a Phospholipid Bilayer: A 10 Microsecond All-Atom Molecular Dynamics Simulation KEN-ICHI NOMURA, AMIT CHOUBEY, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, University of Southern California, Los Angeles, California 90089-0242, USA — Cholesterol (CHOL) molecules play a key role in modulating the rigidity of cell membranes, and controlling intracellular transport and signal transduction. Using all-atom molecular dynamics and the parallel replica approach, we study the effect of CHOL molecules on mechanical stresses across a dipalmitoylphosphatidycholine (DPPC)-CHOL bilayer, and the mechanism by which CHOL molecules migrate from one bilayer leaflet to the other (flip-flop events). On average, we observe a CHOL flip-flop event in half-a-microsecond. Once a CHOL flip-flop event is triggered, the inter-leaflet migration occurs in about 62 nanoseconds. The energy barrier associated with flip-flop events is found to be 73 kJ/mol. Results for membrane rigidity as a function of CHOL concentration will also be presented.

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