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Cholesterol Translocation in a Phospholipid Membrane AMIT CHOUBEY, RAJIV KALIA, Collaboratory for Advanced Computing and Simulations, USC, NOAH MALMSTADT, Mork Family Department of Chemical Engineering and Materials Science, USC, AIICHIRO NAKANO, PRIYA VASHISTHA, Collaboratory for Advanced Computing and Simulations, USC — 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 process of CHOL interleaflet transport (flip-flop) in a dipalmitoylphosphatidycholine (DPPC)–CHOL bilayer, the effect of this process on mechanical stress across the bilayer, and the role of CHOL in inducing molecular order in the respective bilayer leaflets. The simulations are carried out at physiologically relevant CHOL concentration (30%), temperature 323 K and pressure 1 bar. CHOL flip-flop events are observed with a rate constant of 3×10^4 s^{-1}. Once a flip-flop event is triggered, a CHOL molecule takes an average of 73 nanoseconds to migrate from one bilayer leaflet to the other.

Amit Choubey
Collaboratory for Advanced Computing and Simulations, USC

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