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Molecular Transport through Flexible Membranes: Coupling between Solute Dynamics and Membrane Fluctuations[1] YONG NAM AHN, YOUNG-MIN BAN, DMITRY KOPELEVICH, University of Florida — Mechanism of solute transport through self-assembled membranes, such as lipid bilayers and surfactant monolayers, is investigated. It is demonstrated that dynamics of the solute molecule significantly deviates from the Markovian Brownian motion. Specifically, the correlation time of the random force acting on the solute increases by two orders of magnitude within a very narrow (less than 1 nm wide) region within or near the membrane. We demonstrate that the slow fluctuations of the random force in this narrow region are caused by dynamic coupling of the solute transport with the membrane undulations. This coupling is the strongest near a free energy barrier for the solute transport through the membrane. Therefore, the coupling is expected to play significant role in the mass transport through a membrane. A stochastic model for the coupled solute-membrane dynamics is developed using results of molecular dynamics simulations. The observed mechanism appears to be very general and is expected to affect mass transport through other flexible membranes.

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