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Subdiffusion and diffusion of lipid atoms and molecules in phospholipid bilayers ELIJAH FLENNER, Colorado State University, JHUMA DAS, MAIKEL RHEINSTADTER, IOAN KOSZTIN, University of Missouri-Columbia —
We examine the dynamics of lipid atoms and molecules using a 0.1 μs all-atom molecular dynamics simulation of a hydrated diyristoyl-phosphatidycholine (DMPC) lipid bilayer. We identify three well separated time regimes in the mean square displacement, $\langle \delta r^2(t) \rangle$, of the lipid atoms and molecules: (1) a ballistic regime for $t < 10$ femptoseconds; (2) a subdiffusive regime where $\langle \delta r^2(t) \rangle \sim t^\beta$ and $\beta < 1$ for times between 10 picoseconds and 10 nanoseconds; and (3) a Fickian diffusion regime where $\langle \delta r^2(t) \rangle \sim t$ for $t > 30$ nanoseconds. We propose a memory function approach for describing the mean square displacement over the whole time range, and find that the lateral self diffusion coefficient found from the memory function approach agrees well with the one determined from the mean square displacement. We use the cumulant expansion of the self-intermediate scattering function to connect the three time scales in the mean square displacement to the interpretation of neutron scattering signals.

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