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Abstract

Neutrons scatter quasielastically from stochastic, diffusive processes, such as overdamped vibrations, localized diffusion and transitions between energy minima. In biological systems, such as proteins and membranes, these relaxation processes are of considerable physical interest. We review here recent methodological advances and applications of quasielastic neutron scattering (QENS) in biology, concentrating on the role of molecular dynamics simulation in generating data with which neutron profiles can be unambiguously interpreted. We examine the use of massively-parallel computers in calculating scattering functions, and the application of Markov state modeling. The decomposition of MD-derived neutron dynamic susceptibilities is described, and the use of this in combination with NMR spectroscopy. We discuss dynamics at very long times, including approximations to the infinite time mean-square displacement and nonequilibrium aspects of single-protein dynamics. Finally, we examine how neutron scattering and MD can be combined to provide information on lipid nanodomains.

Keywords: Dynamics, Biomolecules, Neutron Scattering, MD simulation