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Using Molecular Dynamics simulations in the analysis of Electron Spin Resonance spectra DENIZ SEZER, Physics Dept., Cornell Univ., BENOIT ROUX, IMPS, IBD, CIS, Univ. of Chicago — ESR spectra from spin labeled sites in proteins are sensitive both to the conformations of the spin label at the labeled site and to its flexibility and rate of transition between multiple conformations. Even though measures of spin label mobility can be extracted directly from the spectrum, deducing the wealth of factors that affect the spectral line shape is impossible in most of the cases. Often, one has to model the motion of the spin label and calculate spectra for different values of the parameters of the model. From the work where this approach has been followed it appears that anisotropic Brownian diffusion in a restricting potential constitutes a good description of the spin label motion. This hydrodynamic depiction correlates poorly with the molecular structure of the spin label and its linker. To address this limitation, we combine MD simulations with stochastic models in the simulation of ESR spectra. This allows us to treat the structure and the fast dynamics of the spin label and its environment in atomistic detail, while handling the slower motional modes to which the spectrum is susceptible phenomenologically. We analyse the MD trajectories with the Redfield formalism, appropriate in the fast motional regime. The exchange between the populated rotamers of the spin label and the overall tumbling of the macromolecule, occurring on a longer time scale, are accounted for using stochastic dynamics.

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