

Abstract Submitted
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Intrinsic Mean Square Displacement in Proteins DERYA VURAL, HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware — The dynamics of biological molecules is investigated in neutron scattering experiments, in molecular dynamics simulations, and using analytical theory. Specifically, the mean square displacement (MSD), $\langle r^2 \rangle_{exp}$, of hydrogen in proteins is determined from measurements of the incoherent elastic neutron scattering intensity (ENSI). The MSD, $\langle r^2 \rangle_{exp}$, is usually obtained from the dependence of the ENSI on the scattering wave vector Q . The MSD increases with increasing temperature reaching large values at room temperature. Large MSD is often associated with and used as an indicator of protein function. The observed MSD, however, depends on the energy resolution of the neutron spectrometer employed. We present a method, a first attempt, to extract the intrinsic MSD of hydrogen in protein from measurements, one that is independent of the instrument resolution. The method consists of a model of the ENSI that contains (1) the intrinsic MSD, (2) the instrument resolution width and (3) a parameter describing the motional processes that contribute to the MSD. Several examples of intrinsic MSDs $\langle r^2 \rangle$ in proteins obtained from fitting to data in the existing literature will be presented.

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