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Multi-time scale functional protein dynamics probed by quasielastic neutron scattering

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Proteins are complex molecular systems whose internal dynamics is characterized by a vast spectrum of time scales, ranging from sub-picoseconds for vibrations of chemical bonds to seconds and beyond for large conformational rearrangements. Using a “minimalistic” multi-time scale model for the relaxation dynamics of proteins~[1,2], we show here that even small changes due to external stress, such as temperature, solvent modification or ligand binding, can be elucidated by quasi-elastic neutron scattering (QENS).
The neutron intermediate scattering function is here written in the form $F(q,t) = EISF(q)+(1-EISF(q))\phi(q,t)$, where $EISF(q)$ is the elastic incoherent structure factor which gives information about the motional amplitudes of the hydrogen-atoms in hydrogen-rich systems, and $\phi(q,t)$ is a relaxation function which is chosen to be the “stretched” Mittag-Leffler function, $\phi(q,t) = E_\alpha(-(t/\tau)^\alpha)$ in order to account for the asymptotically self-similar relaxation dynamics of proteins.
An important technical point is the estimation of the EISF on the basis of its measured counterpart and the model parameters of the relaxation function, which are the q-dependent form parameter α and the time scale parameter τ [3].

Our first example concerns the intrinsically disordered protein Myelin Basic Protein (MBP) in solution, which is studied in pure D_2O-buffer and in a mixture of D_2O-buffer with 30\%\, deuterated Trifluoroethanol at different temperatures, in order to evaluate the impact of formation of secondary structure elements on the internal dynamics [4]. The second example concerns the change of the internal dynamics of myoglobin in solution in presence of denaturing agents, and the third example is devoted to understanding the functional dynamics of the enzyme Phosphoglycerate kinase. Here the model allows for determining unambiguously the amplitude of the inter-domain fluctuations which are important for its catalytic function.

References:
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