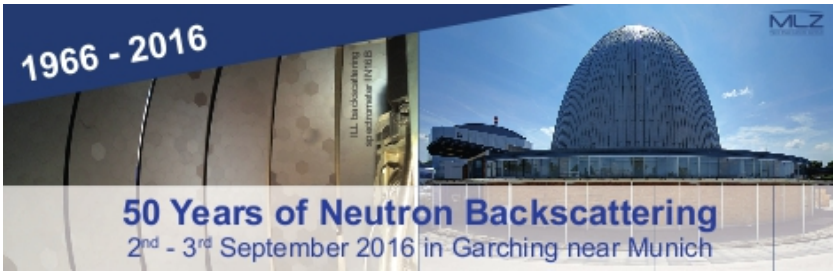

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The Protein Dynamical Transition from Back-Scattering Displacements

Saturday, 3 September 2016 09:35 (20 minutes)

With the fast evolution of molecular dynamic simulations of proteins in the eighties, experimental methods covering structural fluctuations on a picosecond time scale came into focus. Time of flight methods and neutron backscattering provided numerous reality tests of virtual molecular biology. From the experimental side came the idea to expand the physiological range down to low temperatures, to discriminate molecular processes according to the exponential divergence of their correlation times. This approach required total control over the solvent, preventing it from crystallization. Fortunately the solvent could be reduced to a tiny deuterated hydration shell without depressing biological function severely. As a result, the scattering contribution of the protein hydration shell was low and the adsorbed water prevailed in a liquid state even at low temperatures. This concept opened a window to record protein fluctuations within a broad range of time scales (1). One important result was the behaviour of the protein mean square displacements with temperature: Two striking transitions in the T-dependence were observed with hydrated proteins at 180 and 240 K. The second transition requires fully hydrated proteins and was thus termed the PDT. It reflects water-coupled collective motions. Other transitions were assigned to side-chain rotation and fast hydrogen bond fluctuations (1-3).
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2) W. Doster, H. Nakagawa and M.S. Appavou, J. Chem. Phys. 139, 45105 (2013)
3) W. Doster, Critical WebSite: WWW.bioneutron.de

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