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Energy landscape in protein folding and unfolding: A proton NMR study probing the energy landscape in the protein folding and unfolding process

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The microscopic mechanisms taking place in the protein folding and unfolding processes represent an interesting and important open question in many fields of science. The free-energy landscape framework and the possible folding pathways chosen by the many protein residues depend on hydration water and thermodynamic conditions. In this study, we investigate by means of nuclear magnetic resonance spectroscopy, the different trajectories along the protein energy surface explored by different molecular groups of hydrated lysozyme. In detail, we study the folding-unfolding process (both in the irreversible and reversible conditions) by following the temperature evolution of the magnetization for hydrophilic and hydrophobic groups of hydrated lysozyme in different thermal cycles. We find that the hydrophilic (the amide NH) and hydrophobic (methyl CH₃ and methine CH) peptide groups evolve and exhibit different behaviors. In fact, the studied process is characterized by different energetic routes that influence the protein configuration stability that in turn strongly depends on hydration water properties. Indeed, we find that the limit of the protein native state is represented by the water singular temperature that characterizes its compressibility and expansivity and is the origin of the thermodynamical anomalies of its liquid state. Furthermore, we interpret the protein folding/unfolding process in the frame of sol-gel transition driven by water as the cross-linker between different protein peptides, where the temperature of irreversible denaturation corresponds to the percolation threshold temperature. Our results are of general interest for all scientists working in fields on the borderline among physics, biology, chemistry, medicine etc.

Biography

Francesco Mallamace has completed his BE at Messina University in 1973 and became Professor of Physics in 1979. He started his scientific career at Rome La Sapienza on laser experiments related with the theory of coherence of light. Then, he worked on complex systems by studying their thermodynamic properties from the stable to the supercooled regime with different experimental approaches, such as scattering (light and neutron), viscoelasticity, sound propagation and NMR. In all studies, he makes use of the proper model of statistical physics. His current research interests include "Dynamical properties of glass forming materials (molecular or polymeric) on approaching the arrested-glassy state".

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