

Cornell Biophysics Colloquium

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4:30 p.m., 700 Clark Hall

PROTEINS: ENERGY LANDSCAPE, FLUCTUATIONS, AND FUNCTION

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Proteins and glasses can assume a very large number of somewhat different conformations and are described by hierarchically organized energy landscapes. Relaxation and fluctuation processes can be understood as motions in the high-dimensional energy landscapes. In proteins and glasses, at least three different fluctuation processes occur: α and β fluctuations and processes that occur even below mK and are often denoted by TLS or tunnel processes. The α fluctuations can be approximated by the Vogel-Tammann-Fulcher relation, while the β fluctuations appear to follow a conventional Arrhenius law. Both are usually nonexponential in time. There is a fundamental difference between fluctuations in glasses and proteins: In glasses, they are independent of the environment; in proteins they are controlled by it. The α fluctuations in proteins are slaved to the α fluctuations in the solvent surrounding the protein; they follow their rate coefficients but they are entropically slowed. They govern large-scale motions that are important for protein function, such as the exit of small molecules from proteins. The β fluctuations follow the β fluctuations in the protein's hydration shell, a thin layer of water surrounding the protein. They occur even if the environment is solid, but are absent if the hydration layer is removed. They appear to control internal processes in the protein. Understanding the energy landscape, the fluctuations, their structural explanation, and their importance for functions is at present only at a beginning.