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Abstract

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THE ROLE OF WATER IN PROTEIN DYNAMICS

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Without proteins and water, life as we know it would not be possible. Texts and most publications show proteins naked, without a hydration shell and without bulk solvent. Experiments show, however, that the bulk solvent and the hydration shell are essential for proteins to function. What is their role? In particular, how is water involved? Recent experiments have shed some light on these problems using and extending concepts borrowed from the physics of glasses and supercooled liquids (PNAS 106, 5129, 2009). Proteins are dynamic systems; they must fluctuate in order to work. Glasses show two main types of fluctuations, α and β . Proteins and their environment also experience similar fluctuations. The α fluctuations originate in the bulk surrounding and influence the shape of proteins. The β fluctuations originate in the hydration shell, two layers of water around proteins, and control the internal breathing. The role of water and of fluctuations is becoming clearer and the path to further directed experiments is now open.