Roles of Water and ATP in Functioning of ATP-Driven Proteins

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Upon the biological self-assembly, the number of accessible translational configurations of water in the system increases greatly, leading to a large gain in the water entropy. Using our theoretical methods wherein this effect is treated as the key factor, we have succeeded in reproducing the thermodynamic data of apoplastocyanin folding [1], elucidating the pressure [2] and cold [3] denaturation of proteins, suggesting a measure of thermal stability of proteins [4], and developing a free-energy function which is capable of discriminating the native fold from misfolded decoys [5]. The tool is either the three-dimensional integral equation theory [6] or the angle-dependent integral equation theory [7] combined with the morphometric approach [8].

We believe that the water-entropy effect plays critical roles in the functioning of ATP-driven proteins. We have recently made significant progresses in the following subjects: (1) the unidirectional movement of a linear-motor protein along a filament [9]; (2) rotational mechanism of F_1-ATPase [10]; and (3) insertion of an unfoled protein and release of the folded one into and from the chaperonin GroEL [11]. In this talk, I will discuss the roles of water (especially, its translational entropy) coupled with the cycle of the ATP binding, hydrolysis, and release of the products (Pi and ADP) in the functioning of these ATP-driven proteins.

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