Structural investigation of a semi-clathrate hydrate formation using porous ferritin crystals

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Water molecules play essential roles in maintaining the structure and functions in proteins through either hydrogen bonding networks or coordinating to metal centers. Besides such roles, the water molecules can form polynuclear clathrates in antifreeze proteins, such as “maxi,” commonly known as semi-clathrate hydrate[1]. Such unique clathrates in antifreeze protein prevent ice formation in organisms in sub-zero temperature[2]. Artificial development of such semi-clathrate hydrates is an emerging area of research considering potential applications in cryotechnology, including food preservation, organ storage, cryo-medicine, etc. However, limited information about their design, construction, structure, and dynamics in variable temperatures is known.

This presentation will describe the X-ray crystal structures of a single semi-clathrate hydrate structure formation on the surface of the ferritin cage (Figure 1). The semi-clathrate hydrate formation is useful for fundamental understanding and applications. We determined the structures at variable temperatures ranging from -180℃ to 0℃ to explore the formation mechanism of the semi-clathrate hydrate and its stability. In addition, we performed mutational analysis to find out the key residues responsible for the formation and stability of the water cluster networks. Overall, the work is significant not only for fundamental understanding but also for the design and construction of artificial semi-clathrate hydrates on a protein.

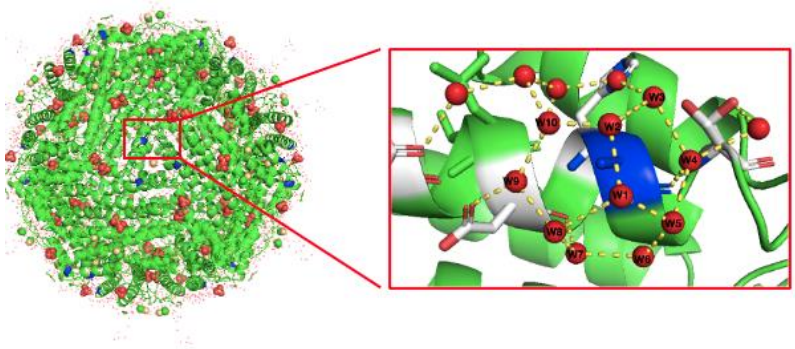

Figure 1. A semi-clathrate water network on the ferritin cage.

Reference:

[1] T. Sun, et al., *Science*. 343, 795-798 (2014)

[2] P. L. Davies, *Trends Biochem. Sci*, 39, 548-555 (2014)