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Metal ion coupled protein folding and allosteric motions[1]

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Many proteins need the help of cofactors for their successful folding and functioning. Metal ions, i.e., Zn^{2+}, Ca^{2+}, and Mg^{2+} etc., are typical biological cofactors. Binding of metal ions can reshape the energy landscapes of proteins, thereby modifying the folding and allosteric motions. For example, such binding may make the intrinsically disordered proteins have funneled energy landscapes, consequently, ensures their spontaneous folding. In addition, the binding may activate certain biological processes by inducing related conformational changes of regulation proteins. However, how the local interactions involving the metal ion binding can induce the global conformational motions of proteins remains elusive. Investigating such question requires multiple models with different details, including quantum mechanics, atomistic models, and coarse grained models. In our recent work, we have been developing such multiscale methods which can reasonably model the metal ion binding induced charge transfer, protonation/deprotonation, and large conformational motions of proteins. With such multiscale model, we elucidated the zinc-binding induced folding mechanism of classical zinc finger and the calcium-binding induced dynamic symmetry breaking in the allosteric motions of calmodulin [1,2]. In addition, we studied the coupling of folding, calcium binding and allosteric motions of calmodulin domains. In this talk, I will introduce the above progresses on the metal ion coupled protein folding and allosteric motions.

[1] Li WF, Zhang J, Wang J, and Wang W, Metal-Coupled Folding of Cys2His2 Zinc-Finger, J. Am. Chem. Soc. 130 (2008) 892-900;
[2] Tan C, Li WF, Wang W, and Thirumalai D, Dynamic symmetry breaking during allosteric transitions in Calmodulin is driven by quantized dehydration of Ca2+ ions, (2013) submitted.

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