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臺灣大學應用力學研究所  
演講公告

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講題：多尺度模擬於生物材料力學易變性之研究探討

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# 多尺度模擬於生物材料力學易變性之研究探討

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## ABSTRACT

Disulfide bonds and metal-coordinate bonds serve as flexible connections on account of their variable bond strength in different chemical environments. Both bonds can act as an effective switch to stabilize or weaken a protein's geometry. These mechanisms are responsible for protein mutability, enabling distinct biological functions. Understanding the bonds' chemistry and mechanics is important for our knowledge of molecular, cellular and tissue level properties of biological materials that contain high ratios of disulfide bonds or metal-coordinate bonds, such as hair and Nereis jaws.

In this study, we develop the first multiscale frame work to study the hierarchical structure of trichocyte keratin proteins with disulfide bonds from a bottom-up approach. Disulfide bonds result in a higher strength and toughness of keratin proteins, suggesting that disulfide bonds play a significant role in achieving its characteristic mechanical properties of trichocyte keratin. In keratin macrofibrils, disulfide crosslinks contribute to the initial modulus and enhance the robustness of macrofibrils by facilitating cooperative deformation of microfibrils at larger deformation.

We also study the mutability of Nvjp-1 protein with metal-coordinate bonds in varied chemical environments from the single molecule level to larger length scales ( $\sim\mu\text{m}$ ). Nvjp-1 forms a more compact structure in the presence of Zn ions with more stable intra-molecular metal coordinate complexes at higher ion concentrations. As pH increases, deprotonation of histidine amino acids weakens the electrostatic repulsion, allowing a greater intramolecular interaction and a shift to a folded conformation. We find that pH also controls the stiffness and modulus of Nvjp-1. This study suggests that the metal-coordinate crosslinks and pH induce significant Nvjp-1 aggregation and achieve the contraction of the Nvjp-1 stripe observed in experiments.