Investigation of Structural and Mechanical Properties of Silk Fibroin and its Applications in Biomedical areas

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Among different species of biomaterials, silk fibroin has attracted great attention due to its superior mechanical properties such as high stretchability, high strength, biocompatibility, as well as its biodegradability.[1] They can be made into various morphologies, for example hydrogels, sponges, films, etc., so as to facilitate their wide applications as surgical sutures, tissue engineering scaffolds, drug carriers, biosensors, etc. Recently, great efforts are demanded in order to understand and further enhance the mechanical properties of silk fibroin in terms of strength and toughness based on molecular level. Carbon-based nanomaterials could effectively reinforce the mechanical properties of silk fibroin. In this study, largescale molecular dynamics simulations were carried out on silk crystalline and the interactions between graphene substrate and model peptides extracted from silk fibroin.[2,3] The simulation result including the energetics of chain-chain interaction, the secondary structure evolution of silk peptides agrees well with the experimental data. Our study shows that graphene substrate has different impact on structural properties of different domains of silk fibroin. Tensile tests were also carried out on representative peptides to measure the mechanical properties of the peptides related to strength and resilience. It was found that the stregnth of the peptides are enhanced upon adsorption to the graphene surface. These results provide in-depth understandings in molecular structure-mechanical property correlation in protein-nanomaterial interface, and will be helpful to future design of bio-inspired materials for biomedical applications.

Key Words: *Silk fibroin, Molecular dynamics simulation, Mechanical property.*

References

(1) Koh, L. D.; **Cheng, Y**.; Teng, C. P.; Khin, Y. W.; Loh, X. J.; Tee, S. Y.; Low, M.; Ye, E.; Yu, H., D.; Zhang, Y. W.; Han, M. Y. Structures, Mechanical Properties and Applications of Silk Fibroin Materials, Prog. Polym. Sci. 2015, 46, 86–110.

(2) **Cheng, Y.,** Koh, L. D., Li, D., Ji, B., Han, M. Y., Zhang, Y. W., On the Strength of β-sheet Crystallites of Bombyx mori Silk Fibroin, Journal of the Royal Society Interface, 11, 20140305 (2014).

(3) **Cheng, Yuan**; Koh, Leng-Duei, Li, Dechang; Ji, Baohua; Zhang, Yingyan; Yeo, Jingjie; Guan, Guijian; Han, Mingyong, Zhang, Yong-Wei, Peptide-Graphene Interactions Enhance the Mechanical Properties of Silk Fibroin ACS Applied Materials & Interfaces, 2015, 7 (39), pp 21787–21796.