Interactions between Silk Fibroin and Graphene Substrate based on Molecular Dynamics Simulations

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Abstract

Silk fibroin has attracted great attention due to its superior mechanical properties such as ultra-high strength and stretchability, biocompatibility, as well as its versatile biodegradability and processability [1]. They can be made into various morphologies such as sponges, hydrogels, films, mats and particles, facilitate their wide applications as apparel/medical textiles, surgical sutures, tissue engineering scaffolds, drug/gene carriers, optics, sensors, etc. Great efforts are demanded in order to further enhance the mechanical properties of silk fibroin. In this study, intensive molecular dynamics simulations were carried out on interactions between graphene substrate and model peptides with different sizes extracted from different domains of silk fibroin. The simulation results on structural properties of silk fibroin agree 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 [2]. 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 of protein upon adsorption to the substrate, and will be significant help to future design of bio-inspired composite materials.

Keywords: *Silk fibroin, Graphene, Molecular dynamics simulation, Mechanical property.*

References

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