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Molecular Dynamics Simulations of Waterborne Biodegradable Polyurethane Hydrogel for 3D Printing

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Biodegradable hydrogels have become popular materials for many biological applications in the past years. They not only exhibit similar mechanical properties as natural soft tissues but also have the ability to be degraded in an aqueous environment after their useful lifetime. Recently, a novel waterborne biodegradable polyurethane (WDPU) has been synthesized and shown to have great potential in biomedical applications. It is synthesized by a green water-based process, and has great biocompatibility, biodegradability, and mechanical properties. Furthermore, it has been used as a 3D printing ink recently to enable the fabrication of biocompatible scaffolds. The integration of biodegradable hydrogel and 3D printing technology has open great opportunities for the design of smart biocompatible scaffolds for many applications due to the ability to access complex internal structures. However, the molecular mechanisms of the self-assembly process of waterborne PUs and the relationship between the chemical compositions of the polymer segments and the material properties of the biodegradable hydrogels are still not clear.

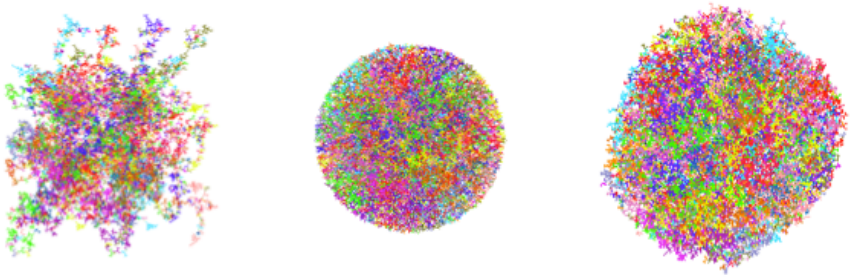

Figure 1. Molecular structure of amorphous WDPU and WDPU nanoparticle.

In this study, we aim to explore the fundamental mechanisms of the WDPU through a full atomistic simulation approach. We use molecular simulations to study the molecular structures of the WDPU containing different soft segments including PCL and PLA. Amorphous unit cells for different WDPU are constructed to study the temperature dependences on the mechanical properties. Furthermore, the WDPU nanoparticles are constructed to study the self-assembly process of the WDPU hydrogel (Figure 1). The end-to-end distances of polymer chains, radius of gyration, and solvent accessible surface area of WDPU nanoparticles are analyzed to investigate the self-assembly behavior, transition temperature, and mechanical properties of WDPU nanoparticles. We find that the material properties of the biodegradable hydrogel can be designed by tuning the molecular weights and the chemical compositions of the polymer segments in the WDPU. Our results provide fundamental insights into

the self-assembly process of WDPU nanoparticles and help enabling the design of material properties of biocompatible hydrogel for future 3D printing applications.