Graduate Student Research Seminar

Spring 2026

Revealing the Plasticization Effect of PHBV on Chitosan in Polymer Blends via Atomistic Simulations

Ji Yang (PhD Student)

Advisor: Zhaoxu Meng

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3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

Chitosan (CS) is a biodegradable, biocompatible, and low-cost biopolymer with broad applications; however, its inherent chain stiffness severely limits its processability. Although numerous plasticizers have been explored to enhance CS flexibility, the potential of poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV), another biodegradable biopolymer, as a plasticizer in CS/PHBV blends remains insufficiently understood, particularly at the molecular level. In this study, we employ atomistic molecular dynamics simulations to systematically investigate the miscibility and plasticization effect of PHBV in CS-based blends. We first examine the molecular-level miscibility of CS and PHBV using Flory-Huggins interaction parameter across a series of blend compositions at both 300 K (service condition) and 500 K (processing condition), revealing favorable miscibility at both temperature regimes, particularly at extreme compositions. Steered molecular dynamics simulations demonstrate that CS chains possess substantially higher backbone stiffness and rigidity than PHBV, underscoring the plasticization potential of PHBV. Two representative blend ratios, 10:90 and 90:10 (PHBV:CS), are examined to probe chain mobility, mechanical response, and conformational flexibility. Results show that PHBV enhances CS chain mobility and ductility under tensile deformation, while CS imposes modest confinement on PHBV dynamics. Dihedral energy analysis further confirms that PHBV facilitates conformational transitions in CS chains, lowering the energetic barriers for deformation. Notably, these plasticization effects persist in a phase-separated model, highlighting the robustness of PHBV's plasticization effect. Collectively, our findings provide molecular-level insights into the dual role of PHBV as both a miscible component and an effective plasticizer in CS-based biopolymer blends, with implications for the design of flexible, processable, and sustainable polymeric materials.

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