Bio-Based Surfactant–Polymer Assemblies for Agrochemical Active Ingredient Release: A Molecular Dynamics Study

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In agrochemical applications, the controlled and targeted release of active ingredients is essential to improve efficacy while minimizing environmental impact. Smart surfactants are emerging as key formulation components because they can respond to external stimuli and trigger the release of active ingredients only under specific environmental conditions. In this work, we investigate the encapsulation of poorly water-soluble active ingredients using mixtures of bio-based smart surfactants and polymers, which self-assemble into mixed aggregates capable of stabilizing hydrophobic compounds in aqueous environments.

Using computational modeling based on Molecular Dynamics, we study how aggregate structure, stability, and compatibility with the encapsulated active ingredient vary as a function of external parameters such as pH and salinity. By linking environmental changes to aggregate stability and disassembly, this work provides mechanistic insight into stimuli-responsive release mechanisms, demonstrating how active ingredients can be released autonomously in response to environmental conditions encountered in agricultural soils. The results support the rational design of smart surfactant–polymer delivery systems aligned with safe-and-sustainable-by-design principles for next-generation agrochemical formulations.

Keywords:
Safe and sustainable by design, molecular dynamics simulations, bio-based surfactants, agrochemical, encapsulation, stimuli-responsive release

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