Unraveling Oil–Water Interfacial Mechanisms in Chitosan-Modified OEG Microgels via Dissipative Particle Dynamics

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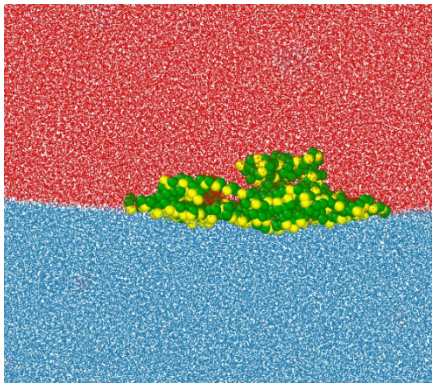
Oligo(ethylene glycol) (OEG)-based microgels have recently emerged as promising alternatives to traditional Poly(N-isopropylacrylamide) (PNIPAM) systems due to their non-toxicity, excellent emulsion stabilization, and robust mechanical properties. Their ability to form soft, stimuli-responsive networks makes them particularly attractive for biomedical and interfacial engineering applications [1]. To further enhance their biocompatibility and functional tunability, OEG microgels can be combined with methacrylated chitosan, a naturally derived, biodegradable polymer known for its intrinsic biocompatibility, antimicrobial activity, and pH-responsive behavior. This combination introduces a new class of fully non-toxic, environmentally benign microgels capable of responding to multiple external stimuli [2].
While OEG/chitosan microgels show promise, their interfacial mechanisms remain unclear due to the limitations of experimental techniques in resolving nanoscale interactions. We address this using Dissipative Particle Dynamics (DPD) simulations, a mesoscopic approach ideal for capturing microgel morphology and interfacial tension [3].
This study uses numerical simulations to investigate the volume behavior, temperature sensitivity, and pH responsiveness of OEG/methacrylated chitosan microgels. By emphasizing their role in oil–water compatibilization, we provide a mechanistic understanding of how chitosan modulates swelling and interfacial anchoring. These findings facilitate the rational design of biocompatible microgels for drug delivery, food emulsions, and eco-friendly formulations.

Keywords:
Microgel, Chitosan, Simulations, Dissipative Particle Dynamics



DPD snapshot of a microgel particle adsorbed at an oil-water interface. The oil (red) and water (blue) phases are clearly seperated, with the microgel beads (yellow/green) flattening into a fried-egg structure.

References:

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