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Modelling Soil-release Polymers on Fabric Surfaces: A Multiscale Study using DPD and Enhanced Sampling MD Simulations

Soil release polymers (SRPs) are amphiphilic polymers found in modern detergent formulations, whose primary operations are to modify synthetic fabric surfaces to allow water transport and to prevent the redeposition of oil-based soil particles during the wash cycle.1 In this work, SRPs are modelled at fabric surface-water interfaces using dissipative particle dynamics (DPD) and Hamiltonian replica exchange molecular dynamics (H-REMD), the latter of which lowers energy barriers to allow us to explore conformations that are outside of the timescale of conventional MD.2

DPD is a mesoscale, coarse-grained modelling technique, that falls on length and time scales somewhere between atomistic simulations and macroscale simulations.3 This makes it ideal for observing mesoscale phenomena at longer timescales, while still retaining some chemical detail. We describe the process of parametrising and validating these simulations and explore how changes in polymer structure affect surface binding and solution aggregation. Combined with enhanced sampling methods (H-REMD and umbrella sampling), we can accurately extract free energy curves to gain a quantitative understanding of the surface-polymer interactions.4 By collaborating with synthetic chemists and industry partners, this work will help in screening for more effective greener candidates.

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