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Design of new polymers for surface modification of fabrics: a multi-scale molecular modelling approach

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Soil-release polymers (SRPs) are important components of fabric care formulations. They play an important role in cleaning by modifying the surface of fabrics such as polyester. SRPs change the surface hydrophobicity, providing resistance to staining and preventing the redeposition of soils during the wash process. They have important environmental benefits, enabling effective cleaning of fabrics while using shorter, cooler wash cycles. This is significant from an environmental perspective as, typically, 10–15% of household energy is used by washing machines, and washing at 30 ℃ rather than 40 ℃ can reduce energy consumption by ˜40% per cycle.

The typical schematic structure of an SRP is shown here. They are traditionally built as tri-block copolymers with two (long) terminal hydrophilic chains designed to impart hydrophilicity to the surface, and a short central hydrophobic block designed to anchor strongly to a fabric surface. Most SRPs used today contain petroleum-sourced terephthalic acid, produced via the catalytic oxidation of petroleum-sourced p-xylene. However, there is a clear drive throughout industry to replace this with non-petroleum-based alternatives [1].

Two factors are known to be important: the binding strength of the central hydrophobic block to the polymer surface and the aggregation behavior of the polymer in solution. Hydrophobic oligomers tend to fold in solution to minimize contact with water, and so (typically) contact between this part of the polymer and the surface occurs in “folded form”. Moreover, there can also be a tendency for aggregate formation to occur in solution, and large aggregates are known not to stick to the fabric surface.

To understand the complex behavior of these polymers, we present a multiscale simulation approach. H-REMD is used to determine the folded structures of molecules in solution, and of the central core at polyester and spandex surfaces. µs MD is used to study initial aggregation behavior in solution and is used to parametrise and validate a dissipative particle dynamics (DPD) model of the polymer. The latter is used to simulate the full solution aggregation and surface adsorption behavior at a hydrophobic interface.

This multi-scale approach has facilitated the design of new biosourced “greener polymers”.

[1] E. F. Fiandra; L. Shaw; M. Starck; C. J. McGurk; C. S. Mahon, Chem. Soc. Rev., 2023, 52, 8085-8105. Designing biodegradable alternatives to commodity polymers. [2] M. Starck; E. F. Fiandra; J. Binks; G. Si; R. Chilton; M. Sivik; R. L. Thompson; J. Li; M. R. Wilson; C. S. Mahon; JACS AU 2025, 5, 666-674. Surface Modification of Polyesters Using Biosourced Soil-Release Polymers.

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