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Investigating the Localization of Dyes within Surfactant Micelles using CV-SANS

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Surfactants are one of the most important product categories in chemical industry. Consumer care is a prominent area in the wide variety of commercial applications. In this study, the localization of dyes within surfactant micelles is studied utilizing small-angle neutron scattering (SANS) combined with contrast variation using deuterated surfactant molecules. Additional NMR measurements helped confirming the localization of dye molecules within the micelles.

In a first step, we characterized the self-assembly behaviour of three commercial azo hair dyes, of blue, yellow and red colour, using a NaHCO3/Na2CO3 buffered solution at pH 10.5 [1]. We could, with UV-vis spectroscopy and SANS, prove that despite their similar chemical nature, the three dyes behave differently: Whereas yellow does not self-aggregate, blue only forms dimeric assemblies, but red aggregates even further, into fractal-like structures which are composed of cylindrical segments.

Dyeing formulations and hair care products contain different types of surfactants. Therefore, we dissolved a dye in solutions of either a cationic (DTAB) [2, 3] or a nonionic surfactant (C12E5) [4]. Micelles formed between dye and the cationic surfactant adopt different morphologies, ranging from short elliptical micelles to wormlike structures, depending on the concentration ratio of dye to surfactant. The dye is located in the outer region of cationic surfactant micelles. Dissolving the dye in a nonionic surfactant solution, both temperature and pH become additional parameters that govern the adopted micellar shapes. The dye localization is seen to depend on the pH, moving from the interior via the palisade to the outer micellar region as the pH is increased.

References
[1] W. Müller et al., Soft Matter 19, 4579 (2023)
[2] W. Müller et al., Soft Matter 19, 4588 (2023)
[3] W. Müller et al. Nanoscale Advances 5, 5367 (2023)
[4] W. Müller et al. Langmuir (2024), in print

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