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H-bonding in acid-glycol switchable emulsifiers enlightened with sum-frequency generation spectroscopy

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Switchable emulsifiers are commonly studied at the macroscopic scale without significant insight into the molecular properties and processes underpinning their behaviour. Our work investigate a switchable emulsifier comprising poly(methacrylic acid) (PMAA) and poly(ethylene glycol) methacrylate (PEGMA). At alkaline pH, the polymer produces stable emulsions with well dispersed droplets, whereas at acidic pH the droplets aggregate. Here, we use sum frequency generation (SFG) spectroscopy to develop a molecular level understanding of the surface of the emulsifier coated droplets. With SFG spectroscopy we basically obtain the vibrational spectrum of an interface. In detail, we monitor the C=O vibration of PMAA as a function of dilution with PEGMA. From the observed changes, it can be concluded that at pH 2.5, both MAA-EG H-bonds and MAA = MAA cyclic dimers contribute to droplet aggregation in the emulsion. In contrast, from SFG spectra in the C-H/O-H stretch region, it can be concluded that at pH 11.5 deprotonation and solvation of the PMAA component lead to a polymer restructuring. As a result, the PMAA chains form a negative shell around the droplets, electrostatically stabilising the emulsion in alkaline conditions. Therefore, we conclude that the behaviour of the polymer is not only due to a simple protonation/deprotonation of the MAA units, but it is a rather complex process involving polymer restructuring, and at least two types of inter-polymer interactions. Our findings not only provide a proof for the so far hypothesised molecular explanation for the behaviour of the PMAA/PEGMA BCS switchable emulsifier, but can also serve as guidance for the design of similar responsive systems with better efficiency in applications ranging from smart materials to drug-delivery.

Keywords

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