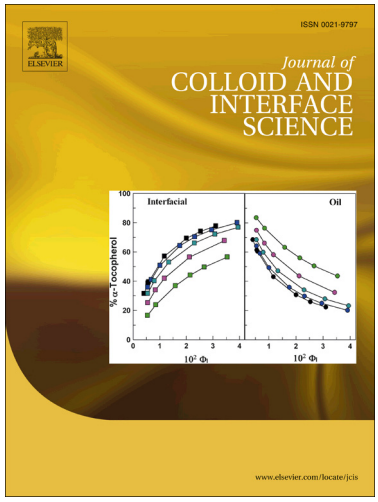

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Modelling the interfacial behaviour of dilute light-switching surfactant solutions

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Abstract

The direct molecular modelling of an aqueous surfactant system at concentrations below the critical micelle concentration (pre-cmc) conditions is unviable in terms of the presently available computational power. Here, we present an alternative that combines experimental information with tractable simulations to interrogate the surface tension changes with composition and the structural behaviour of surfactants at the water-air interface. The methodology is based on the expression of the surface tension as a function of the surfactant surface excess, both in the experiments and in the simulations, allowing direct comparisons to be made. As a proof-of-concept a coarse-grained model of a light switching non-ionic surfactant bearing a photosensitive azobenzene group is considered at the air-