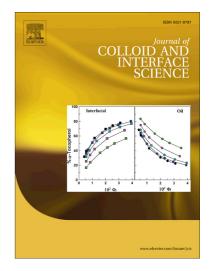
Accepted Manuscript

Modelling the interfacial behaviour of dilute light-switching surfactant solutions

Carmelo Herdes, Erik E. Santiso, Craig James, Julian Eastoe, Erich A. Müller

PII: DOI: Reference:	S0021-9797(14)00993-X http://dx.doi.org/10.1016/j.jcis.2014.12.040 YJCIS 20083
To appear in:	Journal of Colloid and Interface Science
Received Date:	14 October 2014
Accepted Date:	10 December 2014



Please cite this article as: C. Herdes, E.E. Santiso, C. James, J. Eastoe, E.A. Müller, Modelling the interfacial behaviour of dilute light-switching surfactant solutions, *Journal of Colloid and Interface Science* (2014), doi: http://dx.doi.org/10.1016/j.jcis.2014.12.040

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

Modelling the interfacial behaviour of dilute light-switching surfactant solutions

Carmelo Herdes,^a Erik E. Santiso, ^b Craig James, ^c Julian Eastoe ^d and Erich A. Müller^{a,*}

^aDepartment of Chemical Engineering, Imperial College London, London, SW7 2AZ, U.K.

^bDepartment of Chemical and Biomolecular Engineering, North Carolina State University, NC 27695-7905, U.S.A.

^cDepartment of Frontier Materials Chemistry, Graduate School of Science and Technology, Hirosaki University, 3 Bunkyo-cho, Hirosaki, Aomori 036-8561, Japan

^dSchool of Chemistry, University of Bristol, Bristol BS8 1TS, U.K.

* corresponding author: e.muller@imperial.ac.uk

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 airDownload English Version:

https://daneshyari.com/en/article/6997165

Download Persian Version:

https://daneshyari.com/article/6997165

Daneshyari.com