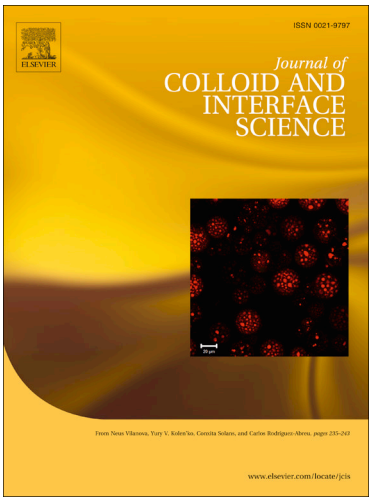

Self-assembly of ellipsoidal particles at fluid-fluid interfaces with an empirical pair potential

Alan M. Luo, Jan Vermant, Patrick Ilg, Zhenkun Zhang, Leonard M.C. Sagis

PII: S0021-9797(18)31037-3
DOI: https://doi.org/10.1016/j.jcis.2018.08.114
Reference: YJCIS 24047

To appear in: *Journal of Colloid and Interface Science*

Received Date: 4 June 2018
Revised Date: 29 August 2018
Accepted Date: 30 August 2018

Please cite this article as: A.M. Luo, J. Vermant, P. Ilg, Z. Zhang, L.M.C. Sagis, Self-assembly of ellipsoidal particles at fluid-fluid interfaces with an empirical pair potential, *Journal of Colloid and Interface Science* (2018), doi: https://doi.org/10.1016/j.jcis.2018.08.114

Self-assembly of ellipsoidal particles at fluid-fluid interfaces with an empirical pair potential

Alan M. Luo, Jan Vermant

ETH Zürich, Department of Materials, CH-8093 Zürich, Switzerland.

Patrick Ilg

School of Mathematical and Physical Sciences, University of Reading, Reading, RG6 6AX, United Kingdom.

Zhenkun Zhang

Institute of Polymer Chemistry, College of Chemistry, Nankai University, Tianjin 300071, China.

Leonard M.C. Sagis

Physics and Physical Chemistry of Foods, Wageningen University, Bornse Weilanden 9, 6708 WG Wageningen, The Netherlands.

Abstract

Colloidal particles adsorbed at fluid-fluid interfaces interact via mechanisms that can be specific to the presence of interfaces, for instance, lateral capillary interactions induced by nonspherical particles. Capillary interactions are highly relevant for self-assembly and the formation of surface microstructures, however, these are very challenging to model due to the multibody nature of capillary interactions. This work pursues a direct comparison between our computational modelling approach and experimental results on surface microstructures formed by ellipsoidal particles. We begin by investigating the accuracy of using pairwise interactions to describe the multibody capillary interaction by contrasting exact two- and three-particle interaction energies and we find that the pairwise approximation appears reasonable for the experimentally relevant configurations studied. We then develop an empirical pair potential and use it in Monte-Carlo type simulations to efficiently model the stucture formation process for relevant particle properties such as aspect ratio, contact angle and surface cover-