Title: Properties of patchy colloidal particles close to a surface: A Monte Carlo and density functional study

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Source: Journal of Chemical Physics

Volume: 137 **Issue:** 8 **Article Number:** 084704 **DOI:** 10.1063/1.4746428 **Published:** Aug 28 2012

Document Type: Article

Language: English

Abstract: We investigate the behavior of a patchy particle model close to a hard-wall via Monte Carlo simulation and density functional theory (DFT). Two DFT approaches, based on the homogeneous and inhomogeneous versions of Wertheim's first order perturbation theory for the association free energy are used. We evaluate, by simulation and theory, the equilibrium bulk phase diagram of the fluid and analyze the surface properties for two isochores, one of which is close to the liquid side of the gas-liquid coexistence curve. We find that the density profile near the wall crosses over from a typical high-temperature adsorption profile to a low-temperature desorption one, for the isochore close to coexistence. We relate this behavior to the properties of the bulk network liquid and find that the theoretical descriptions are reasonably accurate in this regime. At very low temperatures, however, an almost fully bonded network is formed, and the simulations reveal a second adsorption regime which is not captured by DFT. We trace this failure to the neglect of orientational correlations of the particles, which are found to exhibit surface induced orientational order in this regime. (C) 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4746428]

KeyWords Plus: Directional Attractive Forces; Hard-Sphere Fluid; Associating Fluids; Critical-Beavior; Simulation; Coexistence; Model; Crystals; Liquids; Mixture

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Funding:

Funding Agency	Grant Number
Spanish Ministry of Education	EX2009-0121
Comunidad de Madrid, Spain	MODELICO-CM/S2009ESP-1691
Foundation of the Faculty of Sciences of the University of Lisbon	
FCT	PEst-OE/FIS/UI0618/2011 PTDC/FIS/098254/2008
FP7 IRSES Marie-Curie	PIRSES-GA-2010-269181
	ERC-226207-PATCHYCOLLOIDS

Publisher: Amer Inst Physics

Publisher Address: Circulation Fulfillment Div, 2 Huntington Quadrangle , STE 1 N O 1, Melville, NY 11747-4501 USA

ISSN: 0021-9606

Citation: Gnan N, de las Heras D, Tavares J M, da Gama M M T, Sciortino F. Properties of patchy colloidal particles close to a surface: A Monte Carlo and density functional study. Journal of Chemical Physics. 2012; 8 (137).