

**Title:** Computing the phase diagram of binary mixtures: A patchy particle case study

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**Source:** Journal of Chemical Physics **Volume:** 138 **Issue:** 16 **Article Number:** 164904

**DOI:** 10.1063/1.4802026 **Published:** Apr 28 2013

**Document Type:** Article

**Language:** English

**Abstract:** We investigate the phase behaviour of 2D mixtures of bi-functional and three-functional patchy particles and 3D mixtures of bi-functional and tetra-functional patchy particles by means of Monte Carlo simulations and Wertheim theory. We start by computing the critical points of the pure systems and then we investigate how the critical parameters change upon lowering the temperature. We extend the successive umbrella sampling method to mixtures to make it possible to extract information about the phase behaviour of the system at a fixed temperature for the whole range of densities and compositions of interest. (C) 2013 AIP Publishing LLC.

**Keywords Plus:** Directional Attractive Forces; Thermodynamic Perturbation-Theory; Monte-Carlo; Fluids; Transitions; Behavior; Gelation; Model; Hard

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**Funding:**

Funding Agency	Grant Number
Portuguese Foundation for Science and Technology (FCT)	PEstOE/FIS/UI0618/2011 PTDC/FIS/098254/2008
	ERC-226207-PATCHYCOLLOIDS
	ITN-234810-COMPLOIDS

**Publisher:** Amer Inst Physics

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

**ISSN:** 0162-0134

**Citation:** ROVIGATTI, Lorenzo; DE LAS HERAS, Daniel; TAVARES, Jose Maria; TELO DA GAMA, Margarida M.; SCIORTINO, Francesco - Computing the phase diagram of binary mixtures: A patchy particle case study. Journal of Chemical Physics. ISSN 0162-0134. Vol. 138, nr. 16 (2013).