Title: Phase diagrams of binary mixtures of patchy colloids with distinct numbers and types of patches: The empty fluid regime

Author(s): de las Heras, Daniel¹; Tavares, José Maria¹,²; da Gama, Margarida M. Telo¹,³

Source: Journal of Chemical Physics

Volume: 134 Issue: 10 Article Number: 104904

DOI: 10.1063/1.3561396 Published: Mar 14 2011

Document Type: Article

Language: English

Abstract: We investigate the effect of distinct bonding energies on the onset of criticality of low functionality fluid mixtures. We focus on mixtures of particles with two and three patches as this includes the mixture where "empty" fluids were originally reported. In addition to the number of patches, the species differ in the type of patches or bonding sites. For simplicity, we consider that the patches on each species are identical: one species has three patches of type A and the other has two patches of type B. We have found a rich phase behavior with closed miscibility gaps, liquid-liquid demixing, and negative azeotropes. Liquid-liquid demixing was found to pre-empt the "empty" fluid regime, of these mixtures, when the AB bonds are weaker than the AA or BB bonds. By contrast, mixtures in this class exhibit "empty" fluid behavior when the AB bonds are stronger than at least one of the other two. Mixtures with bonding energies $\epsilon_{BB} = \epsilon_{AB}$ and $\epsilon_{AA} < \epsilon_{BB}$, were found to exhibit an unusual negative azeotrope. (C) 2011 American Institute of Physics. [doi:10.1063/1.3561396]

KeyWords Plus: Directional Attractive Forces; Equilibria; Particles; Crystals; Spheres; Sites

Reprint Address: de las Heras, D (reprint author), Univ Lisbon, Ctr Fis Teor & Computac, Ave Prof Gama Pinto 2, P-1749016 Lisbon, Portugal.

Addresses:
1. Univ Lisbon, Ctr Fis Teor & Computac, P-1749016 Lisbon, Portugal
2. Inst Super Engn Lisboa, P-1959007 Lisbon, Portugal
3. Univ Lisbon, Dept Fis, Fac Ciencias, P-1749016 Lisbon, Portugal

E-mail Address: delasheras.daniel@gmail.com; josemaria.castrotavares@gmail.com; margarid@cii.fc.ul.pt

Funding:

<table>
<thead>
<tr>
<th>Funding Agency</th>
<th>Grant Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Portuguese Foundation for Science and Technology (FCT)</td>
<td>POCTI/ISFL/2/618 PTDC/FIS/098254/2008</td>
</tr>
<tr>
<td>Comunidad de Madrid, Spain</td>
<td>MODELICO-CM/S2009ESP-1691</td>
</tr>
<tr>
<td>Spanish Ministry of Education</td>
<td>FIS2008-05865-C02-02 EX2009-0121</td>
</tr>
</tbody>
</table>
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: DE LAS HERAS, Daniel; TAVARES, José Maria; DA GAMA, Margarida M. Telo - Phase diagrams of binary mixtures of patchy colloids with distinct numbers and types of patches: The empty fluid regime. Journal of Chemical Physics. ISSN 0021-9606. Vol. 134, n.º 10 (2011).