Title: Three-dimensional patchy lattice model for empty fluids

Author(s): Almarza, N. G. [1]; **Tavares, J. M.** [2,3]; Noya, E. G. [1]; Gama, M. M. Telo da [2,4]

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Abstract: The phase diagram of a simple model with two patches of type A and ten patches of type B (2A10B) on the face centred cubic lattice has been calculated by simulations and theory. Assuming that there is no interaction between the B patches the behavior of the system can be described in terms of the ratio of the AB and AA interactions, r. Our results show that, similarly to what happens for related off-lattice and two-dimensional lattice models, the liquid-vapor phase equilibria exhibit reentrant behavior for some values of the interaction parameters. However, for the model studied here the liquid-vapor phase equilibria occur for values of r lower than 1/3, a threshold value which was previously thought to be universal for 2AnB models. In addition, the theory predicts that below r = 1/3 (and above a new condensation threshold which is < 1/3) the reentrant liquid-vapor equilibria are so extreme that it exhibits a closed loop with a lower critical point, a very unusual behavior in single-component systems. An order-disorder transition is also observed at higher densities than the liquid-vapor equilibria, which shows that the liquid-vapor reentrancy occurs in an equilibrium region of the phase diagram. These findings may have implications in the understanding of the condensation of dipolar hard spheres given the analogy between that system and the 2AnB models considered here. (C) 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4771591]

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Reprint Address: Almarza, NG (reprint author) - CSIC, Inst Quim Fis Rocasolano, Serrano 119, E-28006 Madrid, Spain.

Addresses:
[1] CSIC, Inst Quim Fis Rocasolano, E-28006 Madrid, Spain
[2] Univ Lisbon, Ctr Fis Teor & Computac, P-1649003 Lisbon, Portuga
[3] Inst Super Engn Lisboa, P-1959007 Lisbon, Portugal
[4] Univ Lisbon, Dept Fis, Fac Ciencias, P-1749016 Lisbon, Portugal

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