Title: Patching up dipoles: can dipolar particles be viewed as patchy colloids?

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Abstract: We investigate whether the liquid-vapour phase transition of strongly dipolar fluids can be understood using a model of patchy colloids. These consist of hard spherical particles with three short-ranged attractive sites (patches) on their surfaces. Two of the patches are of type A and one is of type B. Patches A on a particle may bond either to a patch A or to a patch B on another particle. Formation of an AA (AB) bond lowers the energy by epsilon AA (epsilon AB). In the limit [image omitted], this patchy model exhibits condensation driven by AB-bonds (Y-junctions). Y-junctions are also present in low-density, strongly dipolar fluids, and have been conjectured to play a key role in determining their critical behaviour. We map the dipolar Yukawa hard-sphere (DYHS) fluid onto this 2A + 1B patchy model by requiring that the latter reproduce the correct DYHS critical point as a function of the isotropic interaction strength epsilon Y. This is achieved for sensible values of epsilon AB and the bond volumes. Results for the internal energy and the particle coordination number are in qualitative agreement with simulations of DYHSs. Finally, by taking the limit [image omitted], we arrive at a new estimate for the critical point of the dipolar hard-sphere fluid, which agrees with extrapolations from simulation.

Author Keywords: Liquid-Vapour Transition; Self-Assembly; Magnetic Fluids

KeyWords Plus: Directional Attractive Forces; Liquid-Vapor Coexistence; Hard-Sphere Fluid; Low-Densities; Phase; Thermodynamics; Sites; Polar

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