Title: Branching points in the low-temperature dipolar hard sphere fluid

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Abstract: In this contribution, we investigate the low-temperature, low-density behaviour of dipolar hard-sphere (DHS) particles, i.e., hard spheres with dipoles embedded in their centre. We aim at describing the DHS fluid in terms of a network of chains and rings (the fundamental clusters) held together by branching points (defects) of different nature. We first introduce a systematic way of classifying inter-cluster connections according to their topology, and then employ this classification to analyse the geometric and thermodynamic properties of each class of defects, as extracted from state-of-the-art equilibrium Monte Carlo simulations. By computing the average density and energetic cost of each defect class, we find that the relevant contribution to inter-cluster interactions is indeed provided by (rare) three-way junctions and by four-way junctions arising from parallel or anti-parallel locally linear aggregates. All other (numerous) defects are either intra-cluster or associated to low cluster-cluster interaction energies, suggesting that these defects do not play a significant part in the thermodynamic description of the self-assembly processes of dipolar hard spheres. (C) 2013 AIP Publishing LLC.

KeyWords Plus: Liquid-Phase, Monte-Carlo; Gas; Ferrofluids; Transition; Particles; Clusters; Colloids

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