Title: Phase diagrams of particles with dissimilar patches: X-junctions and Y-junctions

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Abstract: We use Wertheim's first-order perturbation theory to investigate the phase behaviour and the structure of coexisting fluid phases for a model of patchy particles with dissimilar patches (two patches of type A and f(B) patches of type B). A patch of type alpha = {A, B} can bond to a patch of type beta = {A, B} in a volume nu(alpha beta), thereby decreasing the internal energy by epsilon(alpha beta). We analyse the range of model parameters where AB bonds, or Y-junctions, are energetically disfavoured (epsilon(AB) < epsilon(AA)/2) but entropically favoured (nu(AB) >> nu(alpha alpha)), and BB bonds, or X-junctions, are energetically favoured (epsilon(BB) > 0). We show that, for low values of epsilon(BB)/epsilon(AA), the phase diagram has three different regions: (i) close to the critical temperature a low-density liquid composed of long chains and rich in Y-junctions coexists with a vapour of chains; (ii) at intermediate temperatures there is coexistence between a vapour of short chains and a liquid of very long chains with X-and Y-junctions; (iii) at low temperatures an ideal gas coexists with a high-density liquid with all possible AA and BB bonds formed. It is also shown that in region (i) the liquid binodal is reentrant (its density decreases with decreasing temperature) for the lower values of epsilon(BB)/epsilon(AA). The existence of these three regions is a consequence of the competition between the formation of X- and Y-junctions: X-junctions are energetically favoured and thus dominate at low temperatures, whereas Y-junctions are entropically favoured and dominate at higher temperatures.

KeyWords Plus: Dipolar Particles; Fluids; Sites

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