Title: Re-entrant phase behaviour of network fluids: A patchy particle model with temperature-dependent valence

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Abstract: We study a model consisting of particles with dissimilar bonding sites ("patches"), which exhibits self-assembly into chains connected by Y-junctions, and investigate its phase behaviour by both simulations and theory. We show that, as the energy cost epsilon(j) of forming Y-junctions increases, the extent of the liquid-vapour coexistence region at lower temperatures and densities is reduced. The phase diagram thus acquires a characteristic "pinched" shape in which the liquid branch density decreases as the temperature is lowered. To our knowledge, this is the first model in which the predicted topological phase transition between a fluid composed of short chains and a fluid rich in Y-junctions is actually observed. Above a certain threshold for epsilon(j), condensation ceases to exist because the entropy gain of forming Y-junctions can no longer offset their energy cost. We also show that the properties of these phase diagrams can be understood in terms of a temperature-dependent effective valence of the patchy particles. (C) 2011 American Institute of Physics. [doi: 10.1063/1.3605703]

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