

Title: Computing the phase diagram of binary mixtures: A patchy particle case study

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Abstract: We investigate the phase behaviour of 2D mixtures of bi-functional and three-functional patchy particles and 3D mixtures of bi-functional and tetra-functional patchy particles by means of Monte Carlo simulations and Wertheim theory. We start by computing the critical points of the pure systems and then we investigate how the critical parameters change upon lowering the temperature. We extend the successive umbrella sampling method to mixtures to make it possible to extract information about the phase behaviour of the system at a fixed temperature for the whole range of densities and compositions of interest. (C) 2013 AIP Publishing LLC.

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