

Determination of favorable inter-particle interactions for formation of substitutionally ordered solid phases from a binary mixture of oppositely charged colloidal suspensions

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The solid phase formed by a binary mixture of oppositely charged colloidal particles can be either substitutionally ordered or substitutionally disordered depending on the nature and strength of interactions among the particles. In this work, we use Monte Carlo molecular simulations along with the Gibbs-Duhem integration technique to map out the favorable inter-particle interactions for the formation of substitutionally ordered crystalline phases from a fluid phase. The inter-particle interactions are modeled using the hard core Yukawa potential but the method can be easily extended to other systems of interest. The study obtains a map of interactions depicting regions indicating the type of the crystalline aggregate that forms upon phase transition. © 2013 AIP Publishing LLC.

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