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Liquid-Vapor Like Phase Transition in DNA-Coated Colloids
FRANCISCO MARTINEZ-VERACOECHEA, DAAN FRENKEL, Chemistry Department, University of Cambridge — Colloidal particles coated with DNA-molecules can be designed to bind with high specificity. The result is an unprecedented flexibility for the design of self-assembling systems. Specific interactions can be used to mimic chemical systems at the colloidal level, virtually opening a window to the re-invention of chemistry at a totally new length-scale. Molecular simulations are expected to play a decisive role in the understanding of these materials. In the present work, we use advanced Monte Carlo simulations to study binary systems of DNA-coated colloids, wherein a given type of DNA can only bind to DNA of the opposite type. The system is represented using a coarse-grained model where the DNA interacts through soft-repulsive potentials while the colloids present hard-core interactions only. Binding between DNA is modeled as a harmonic spring between the center of masses of the DNA-chains. The systems are observed to undergo a liquid-vapor like transition for systems where the number of DNA chains per colloid is equal or greater than three. The phase transition is shown to be driven by the entropy gain in bond re-arrangements when the dimers observed in dilute phase form the percolating network typical of the dense phase.

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