Structures in a 2D colloids interacting via modified inverse-power potentials with tunable softening of inner core

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We have used classical density functional theory, HNC integral equation theory (IET) and NVT Monte-Carlo Simulation to investigated the effects of gradual softening of inverse-power repulsive interaction on the pair structure and phase transition properties of the two-dimensional system of colloidal dispersion. We aim to understand the anomalous behaviors and structure formation in a one-component 2D colloidal system using DFT by carefully examining the crossover from one-length to two-length scale characteristics of purely repulsive interaction potential. The particles are assumed to interact via modified inverse-power (MIP) potentials whose strength of the repulsion is softened in a range of distances with an interparticle separation dependent exponent. The radial distribution curves of IET are found to exhibit a non-monotonous nature with an emergence of new peak at a shorter distance. It points to the existence of two competing length scales of nearest-neighbor distance, i.e., a larger soft length fading out with increasing density in favor of the smaller hard length. At higher densities, in-contrast to the HNC IET, the RDF, obtained by MC simulation for high-softness parameter case, display a splitting of the second peak. Using DFT with structural inputs obtained by HNC IET we propose a fluid-triangular solid phase diagram in the temperature-density plane for various softness of the interparticle interaction. Comparison of the virial pressure obtained by HNC and MC simulations has been found to reveal an interesting feature. Whereas the pressure versus density curve given by HNC increases monotonically, the same due to MC simulation, on the other had, shows a discontinuity. Interestingly the line emerging at the discontinuity is found to have greater slope than the line corresponding to fluid. This suggest the possibility of the formation of amorphous glassy phase in 2D system at hand. In order to verify it further, Wendt-Abraham parameter which is a simple and yet useful empirical criterion that has been employed from both the Monte Carlo (MC) and molecular-dynamics (MD) simulations to investigate the liquid-glass transition, has been calculated. We have also calculated the bond orientational order parameter which reaffirms the presence of amorphous solid phase for the case of high softening parameter.