Two-dimensional ordering of nanoparticle dumbbells with charge and size anisotropy: Effects of the electrostatic screening and the size ratio

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I. INTRODUCTION

Formation and controlled growth of ordered phases on a surface is of great interest in electronics research and development. The self assembly of many different nanoparticle systems have been extensively studied and advances in nanoparticle synthesis techniques over the past decade have allowed for the creation of ever more complex multi-meric nanoparticle units, such as dimers and trimers.

II. SIMULATION DETAILS

A. Model

Model dumbbells were composed of two particles of radius R_1 and R_2 respectively and equal but opposite charges. The particles within a dumbbell were held together by a rigid bond of length $L_B = R_1 + R_2$. The inter-molecular interactions between dumbbell particles were modeled by pairwise additive interactions including colloidal and screened electrostatic terms similar to those used by Mani et al.[1]. The colloidal portion of the potential is taken as

$$U_{C,ij} = 4\epsilon \left[(D_{ij}/r_{ij})^{100} - (D_{ij}/r_{ij})^{50} \right] \tag{1}$$

where ϵ is the energy pre-factor denoting the interaction strength and D_{ij} is the effective interaction diameter taken as $D_{ij} = (R_i + R_j)$. The screened electrostatics portion of the potential were taken as

$$U_{E,ij} = \frac{A_{ij}}{\kappa r_{ij}} e^{-\kappa r_{ij}} \tag{2}$$

where κ is the inverse screening distance and A_{ij} is the energetic pre-factor related to the surface potential of the colloidal particles. The interaction potentials were truncated at cutoff distances of $2D_{ij}$ for colloidal and $4D_{ij}/\kappa$ for screened electrostatic interactions. The simulations were run in reduced units where the energy is reduced by ϵ and the distance by R_1. The value of A_{ij} for like charges was taken as 1.0 and was taken as -1.0 for opposing charges. Simulations were run with eight dumbbells in a hard cubic box with number density 0.04. Four different radius ratios $d = R_1/R_2$ were studied including 1.0, 1.359, 1.5, and 2.0. For each d Nested Sampling (NS) simulations were run at various various κ values while all other interaction parameters were held constant.

B. Nested Sampling

Nested Sampling (NS) was originally developed in the context of Bayesian computation by Skilling[2,3] to efficiently compute the evidence of high dimensional spaces where the bulk of the probability is located in exponentially small regions. In the context of atomic systems, NS is an athermal simulation method which allows for the direct computation of the partition function while effortlessly handling phase transitions. We have used a slightly modified version of the multiple walker NS demonstrated by by Pártay et al.[4] Initial simulations were run at select κ values with the number of sample walkers as $K = 4001$. However, several of these were subsequently identified as interesting transition regions and were re-run with $K = 6001$. Additional κ values were also added around points of interest with $K = 6001$. We took the fixed nested cutting fraction to be $f = 1/2$, rather than $K/(K + 1)$ as used by by Pártay et al.[4] For each κ value three independent simulations were run, the expectation values averaged for the three simulations, and the error bars taken as the standard deviation.

C. Molecular Dynamics

III. RESULTS AND DISCUSSION

IV. CONCLUSIONS

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