Interaction Between Nanoparticles Mediated by Grafted Chains

D. Duque[C,S]
Departamento de Fisica Teorica de la Mat. Cond, Universidad Autonoma de Madrid, Madrid, Spain
daniel.duque@uam.es

L.F. Vega
Molecular Simulation Group, Institut de Ciencia de Materials de Barcelona, Consejo Superior de Investigaciones Cientificas, Bellaterra, Barcelona, Spain

The stability of a colloidal dispersion of nanoparticles is primarily controlled by the interaction between them. This interaction can be greatly altered by coating the nanoparticles with end-grafted molecules. In particular, a colloidal suspension can be thus stabilised against flocculation by the coating-mediated forces. Applications include dispersion and emulsion polymerization in supercritical carbon dioxide, microparticle formation in spray processes, and emulsion stabilization. Despite the practical importance of these coatings, there have been few approaches to this problem from a molecular modelling perspective. Following the pioneering work of Murat and Grest [1] and of Carson Meredith et al. [2], we have carried out molecular simulations of these systems using a configurational bias Monte Carlo method. As a first step, we have obtained results for simplified models that had been proposed in order to introduce some relevant features, such as the effect of a bad solvent (attractive interactions between polymers.) This has led to conclusions of technical interest when simulating these systems, such as how to deal with the grafting of the ends [3]. We have then studied more realistic systems, with the appropriate force fields. In this presentation we will summarize our main results for different nanoparticle materials, grafted molecules and solvents. A systematic study of the influence of physical parameters (temperature, surface coverage, pressure, etc) on the stability of the suspension has also been performed and results will be discussed here.

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