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Triangle-Based Numerical Techniques for the Study of Anisotropic Colloids

The availability of new anisotropic colloidal building blocks (e.g. [4]) has necessitated the development of novel numerical algorithms to help predict the experimentally observed phenomenology using theory and simulations. In this talk, we present results obtained by two such methods, both based on the tessellation of objects with triangles.

Firstly, we study the adsorption of an anisotropic colloid at a liquid-liquid interface using a Pieranski-type free-energy argument. In our approximation free energy of adsorption can be easily determined by approximating the surface area of the colloid using triangles to determine the respective contact areas and contact line lengths [1]. From the free-energy landscape a time-dependent adsorption mechanism can be inferred [2]. Our results give insight into the orientational transitions found in systems of adsorbed cylindrical colloids. In future studies our analysis may be extended to include a wider range of interfacial characteristics.

Secondly, we consider Monte Carlo simulations of hard (non)convex faceted particles. In this case the overlap algorithm is based on covering the surface of the particle with triangles. Using this overlap algorithm we developed an algorithm capable of predicting the densest packing of polyhedral particles and to predict the crystal structure of complex colloids at finite pressure [3]. We also use our method to analyse the self-assembly of octapod-shaped nanocrystals in solution [4]. By combining experimental, simulation, and theory results we were able explain the mechanism behind the experimentally observed aggregation of these octapods into interlocked chains and 3D superstructures. The self-assembly process is driven solely by the shape of the octapod and the directional van-der-Waals forces this effects.

We anticipate our investigation to be the starting point of a more extensive exploration of non-convex colloid and nanoparticle systems.

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