Phase Behaviour and Self-Assembly of Inverse Patchy Colloids

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In the last few years the theoretical investigation of the phase behaviour of particles either with anisotropic shapes or interactions has been a very active field of research. Initially this work was motivated by advances in colloidal science that allowed the synthesis of those particles and that lead to the suggestion of building new materials with the desired properties using a "bottom-up" approach, i.e. by designing the particles that would self-assemble into the target structure[1,2]. However it soon became evident that the theoretical study of those particles was interesting also from a fundamental point of view. Anisotropic particles can exhibit an amazingly reach and unusal phase behaviour[3]. Here we investigate the phase behaviour of Inverse Patchy Particles (IPC), a model representative of negatively charged particles with two positively charged patches at the poles[4]. As a consequence regions with opposite charge attract each other but regions with like charge repel each other. The equilibrium phase diagram was evaluated using a combination of two well established techniques: first, an efficient optimization tool based on ideas of evolutionary algorithm is used to identify the stable structures at zero temperature and, second, the stability of those phases at finite temperature is investigated by free energy calculations[5]. We found that the competition between the attractive and repulsive interactions leads to a wealth of ordered structures, including a laminar structure that is stable over a quite broad region of the phase diagram.

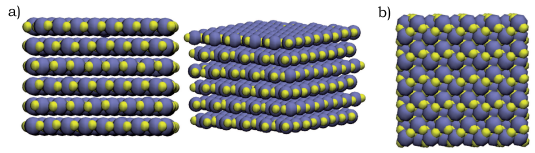

FIG. 1. Two examples of ordered structures formed by IPC particles.

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