# Computation of the phase diagram of simple anisotropic models: patchy and inverse patchy particles

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The recent progress in colloidal science has made it possible to synthesize particles with a tremendous variety of shapes and/or anisotropic interactions, opening novel routes to build new materials with the desired structure and properties by self-assembly of particles with the appropriate interactions [1]. However, the success of this approach relies on our ability to understand how the specific features of the interparticle interactions affect their self-assembly behaviour, an issue where molecular simulation can be a very useful tool.

In this contribution we demonstrate that the phase behaviour of particles with heterogeneously decorated surfaces, so-called patchy particles, can be investigated by a combination of two simulation methods: 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 candidate phases at finite temperature is investigated by free energy calculations [2]. The usefulness of that approach is illustrated with two, highly timely examples. First, the self-assembly behaviour of particles with four patches whose tetrahedral arrangement was varied in a controlled way has been investigated systematically, demonstrating the extremely broad variety of self-assembly scenarios and the ensuing rich phase behaviour of this type of particles [3]. Additionally, we discuss the phase diagram of so-called inverse patchy colloids, a model representative of negatively charged spherical colloids with two positively charged polar patches; as a consequence regions of like charge repel each other, while areas of unlike charges attract each other. The complex competition between the strongly orientational attractive and repulsive interactions leads to the stabilization of a structure formed by a stack of weakly interacting hexagonal layers at low pressures and temperatures, which at high pressure transforms into close packed structures.

[1] Bianchi *et al.* PCCP **13**, 6397 (2001); Anwar *et al.,* Macromol. Rapid Comm. **31**, 150 (2010).
[2] Doppelbauer *et al.* J. Phys.: Condens. Matter **22**, 104105 (2010), Vega, *et al.*, ibid **20**, 153101 (2008).
[3] Doppelbauer *et al.*, Soft Matter **8**, 7768 (2012).