A simple model for the aggregation of chromonic molecules

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Chromonic mesogens are non-conventional amphiphiles, which self-assemble in aqueous solution to form aggregate structures: rods, stacks or layers. These aggregates can subsequently self-organise to form chromonic mesophases. Initial self-assembly is strikingly different to that seen in most conventional amphiphiles: typically being promoted by the interaction of aromatic ring systems and taking place in the absence of a critical micelle concentration. The driving force for chromonic aggregation is hotly debated. For different chromonic systems, static charges, polar and quadrupolar interactions, microphase segregation and entropic contributions to the hydrophobic effect have all been claimed to be significant.

In this presentation we show that a chromonic molecule can be represented by a disk with attractive and repulsive areas of interaction to mimic quadrupolar stacking. Simplifying a molecule in this manner allows for the reproduction of many of the aggregation properties seen in real chromonics; explaining the variation of binding with concentration and the formation of helically ordered aggregates.

The shape of the disks can be distorted to better represent specific molecules, demonstrating how small changes in chemical structure can lead to dramatic differences in aggregation behaviour. Results from this simple model show a remarkable agreement with the predictions from atomistic simulation studies of chromonic disks in aqueous solution.

Figure 1: The interaction between two circular chromonic molecules can be represented as a series of overlaps of attractive and repulsive regions of two disks. Using these overlaps we can predict the most favourable stacking configuration and demonstrate how small chemical changes are reflected in changes in aggregation.

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