Self-assembly of gapped DNA duplexes

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Liquid crystalline phases of double-stranded DNA in aqueous solutions have been studied comprehensively in the past [1-4]. However, so far no smectic phase was observed in DNA duplexes. Here, we show that introducing a flexible single-stranded region into double-stranded DNA can lead to smectic ordering. This finding is indeed surprising, since it's known that flexibility destabilizes layer-like ordering in lyotropic systems. Gapped DNA duplexes- two double-stranded DNA fragments connected with a single-stranded flexible DNA spacer- were found to form an unconventional folded type of smectic mesophase. The smectic layers form due to folding of flexible parts in duplexes and end-to-end stacking interactions between their blunt ends. The folding scenario was backed up by Monte Carlo simulations which highlight that folded smectic phase is thermodynamically stabilized both from entropic and enthalpic point of view [4]. Furthermore, preliminary results demonstrating the impact of suppressed blunt-end attractive interactions on formation of smectic phase will be shown. These results unveil the DNA as a molecular tool which offers numerous possibilities for engineering of lyotropic liquid crystals.

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