Coarse-Grained DNA Modeling

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Development of a Coarse-Grained DNA Model for Bio-Nano-Interfaces

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Background

- DNA is used in a wide variety of applications and technologies including: DNA-based nanomaterials, recognition and separation of carbon nanotubes, biosensors and microarrays, and gene delivery.
- Fundamental understanding at the molecular level of the underlying phenomena is lacking, which negatively impacts our ability to control the outcome thus leaving potential for improvement which can be achieved by modeling.
- In terms of accuracy, all-atom force fields would be most appropriate, but they are not feasible for the length- and time-scales of interest for this system involving large intra- and inter-strand structural rearrangements and involving a large number of components (several DNA strands, SWCNT, solvent, and ions).
- Coarse-grained (CG) DNA models (with fewer degrees of freedom) can provide an alternative representation capable of simplifying the system.

Motivation

- Current models lack necessary properties to model DNA interactions at an interface.
- It is necessary to capture the effect of non-Watson-Crick base pair interactions which play a dominant role in interactions at surfaces.
- Current models lack the ability to simulate many strands.
- Fundamental understanding leads to predictive modeling to better technologies.

Model Outline

The plot shows that the model captures the thermodynamic properties of the duplexes, but not of the hairpins. For future applications, anisotropic hydrogen bonds must be implemented to prevent strand aggregation which should improve the thermodynamics of the hairpins. For the surface interactions of interest, non-Watson-Crick hydrogen bonds play a significant role and must be included as well.

References

2. Boyer, Ding, and Mittal. Journal of Chemical Physics (To Be Submitted).