DNA structures and excited states:

TT photodimerization and DNA-linked nanoparticles

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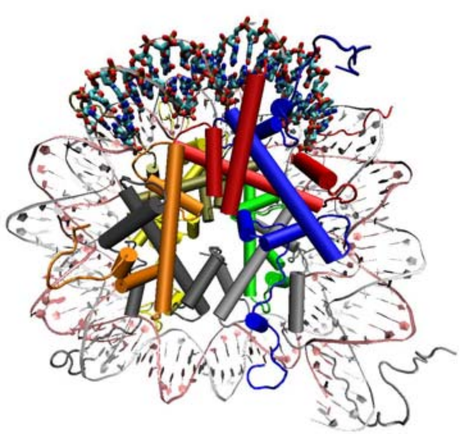

Figure1. Crystal structure of DNA in a nucleosome.

One of the fascinating properties of DNA is that it can either be a small molecule, with just a few base pairs, or it can be a very long polymer, such as in the cell nucleus. In this talk I will describe our recent work on DNA that transitions from small molecule to extended polymer behavior for a number of structural and optical properties. The talk begins with our attempts to understand the structures and absorption spectra of DNA-hairpins, where we show that classical molecular dynamics with standard force fields such as Amber or Charmm provides a remarkably accurate description of many experiments. I then switch to TT photodimerization, which is an important photochemical degradation mechanism in DNA. Here my group has developed a model which makes it possible to determine which TT steps with either single or double stranded structures are most likely to undergo dimerization. We test this model with a number of oligo and hairpin structures, and we describe our attempts at understanding how these effects work with genomic DNA (Fig. 1) that is wrapped around nucleosomes. As another application, I describe several recent studies aimed at understanding how DNA binds to gold nanoparticles, and how it links nanoparticles together to make aggregates and crystalline superlattices (Fig. 2).

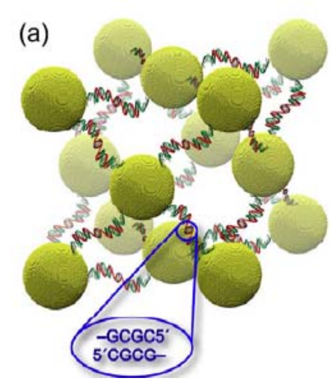

Figure 2. Schematic of DNA-linked gold nanoparticles superlattice.