Synthetic DNAs: Their Structural, Electronic and Conductivity Properties

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Recently, synthetic biologists have been able to synthesize unnatural DNA bases and use them to probe fundamental aspects of biology[1] and make inroads in the creation of artificial genetic systems[2]. Kool's group represents a prominent example of this type of research. This group has embarked in a program to test the limits of size in the DNA backbone and in the proteins that process or bind to DNA. For this purpose DNA base analogues that are larger than their natural counterpart, yet retain the hydrogen bonding capacity, are used. xDNA (short for expanded DNA), is one of the three types of synthetic duplexes that have made with such unnatural bases.

We recently became interested in the possibility of using xDNA for molecular wire applications. Our interest was sparked when we noticed that the melting point of xDNA is, in general, larger than that of their natural counterparts (B-DNA). This fact has been explained, both theoretically and experimentally, as due to xDNA having stronger π-π stacking interactions than B-DNA. As these interactions are believed to play a prominent role in the conductivity process, stands a reason that xDNA could conduct better than B-DNA. This led us to establish a program to elucidate the electronic and conductivity properties of xDNA, and other synthetic DNAs.

In this work, we present a series of *ab initio* results on the structural, electronic and conductivity properties of size-expanded DNA bases and xDNAs duplexes. We show that the size-expanded bases not only have smaller HOMO-LUMO gaps than their natural counterparts, but also that the gaps might be tunable by means of suitable chemical modifications[3a,b,c]. Furthermore, given the same sequence, xDNA duplexes have smaller HOMO-LUMO gaps than their natural counterparts. Preliminary results concerning the conductivity properties of natural and expanded duplexes are also presented.

Taken as a whole, our results indicate that the emerging field of Synthetic Biology, in its ability to create synthetic DNA molecules, might offer viable alternative molecules to DNA for molecular wire applications.

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