Conference: From DNA-Inspired Physics to Physics-Inspired Biology

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Electrostatic Interactions between DNA Double Helices

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Electrostatic interactions between DNA double helices

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Electrostatic interactions between DNA double helices

Predatory adaptation and evolution

Animals - speed  Humans - endurance
Electrostatic interactions between DNA double helices

Homologous pairing  DNA packing  Poly- and meso-morphism
Surface charge pattern

DNA charged helix charged cylinder with counterions
DNA structure and interactions

\[ I(k) = \sum_{v, \mu} \sum_{i,j} f_i f_j \langle F_i^v(k) F_j^\mu(-k) \rangle \]

\[ F_i^v(k) = \frac{1}{(2\pi)^{3/2}} \int n_i^v(r) \exp(ikr) d^3r \]

\[ E \approx \frac{2\pi e^2}{\varepsilon} \sum_{v, \mu=1}^{2} \sum_{i,j} q_i q_j \int \frac{F_i^{T,v}(k) F_j^\mu(-k)}{k^2 + \kappa_D^2} d^3k \]

- ideal, parallel helices (1997)
- ideal, crossed helices (2000)
- straight, non-ideal helices (2004)
- fluctuating helices (ongoing) (static and dynamic torsional, stretching and bending fluctuations)
- counterion correlations (ongoing) (ideal helices, point counterions, no hydrogen bonding, simple limiting cases)

Franklin & Gosling, Nature 171 (1953) 740
Helix-helix alignment

Prediction: Electrostatic interactions cause alignment of DNA backbones in hydrated aggregates

“It therefore seems reasonable to suppose that in structure B the structural units [...] are relatively free from the influence of neighboring molecules, each unit being shielded by a sheath of water.”

Franklin & Gosling, Nature (1953)
Franklin & Gosling were wrong.

But, how do non-ideal, fluctuating helices align?

Homologous pairing of dsDNA

Double stranded DNA (dsDNA) have an innate homology recognition ability

Cherstvy, Kornyshev & Leikin, J. Phys. Chem., 2004

Experiment: Inoue, Sugiyama, Travers, Ohyama, Biochemistry, 2007
Prentiss et al. (this meeting)
Rationalization of measured forces

Undulations of DNA dramatically enhance and extend the range of structure-dependent forces.

\[ \frac{E_{\text{undulations}}}{E_0} \sim \exp\left(\frac{d^2}{\lambda^2}\right) \]

Chiral interactions, cholesteric phase, poly- and meso-morphism

<table>
<thead>
<tr>
<th>blue phases (precholesteric stages)</th>
<th>cholesteric phase</th>
<th>2D columnar hexagonal phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d &gt; 49 \text{ Å}$</td>
<td>$49 \text{ Å} &gt; d &gt; 22 \text{ Å}$</td>
<td>$31.5 \text{ Å} &gt; d &gt; 29 \text{ Å}$</td>
</tr>
<tr>
<td>$C &lt; 160 \text{ mg/ml}$</td>
<td>$160 \text{ mg/ml} &lt; C &lt; 380 \text{ mg/ml}$</td>
<td>$380 \text{ mg/ml} &lt; C &lt; 447 \text{ mg/ml}$</td>
</tr>
<tr>
<td>$\alpha = 2^\circ$</td>
<td>$0.7^\circ &gt; \alpha &gt; 0.46^\circ$</td>
<td>$\alpha = 0$</td>
</tr>
</tbody>
</table>


**Experiment:** Stanley, Hong & Strey, Biophys. J., 2005

Fig. 25. Geometrical configurations as a function of DNA concentration in the different liquid crystalline phases. The concentration $C$ was calculated from the interhelix distances $d$ measured by X-ray diffraction experiments (Durand et al. 1992). The twist angle $\alpha$ was deduced from the cholesteric pitch $P$ (0.5 µm in blue phases and 2.5 µm in the cholesteric) and the interhelix distance $d$. 
Counter-Ion Specific Aggregation

Cherstvy, Kornyshev & Leikin, J. Phys. Chem., 2004
Main conclusions

Helical structure of sugar-phosphate backbone strongly affects interactions between DNA. Conversely, interactions affect the structure of DNA in assemblies.

Static and dynamic undulations strongly enhance and extend the range of the structure-dependent forces. Torsional and stretching fluctuations affect these forces relatively weakly.

dsDNA have an innate ability to recognize sequence homology through electrostatic interactions due to sequence dependence of the DNA backbone structure.
Does direct sequence homology recognition between dsDNA occur *in vivo* and what is its role in homologous recombination?