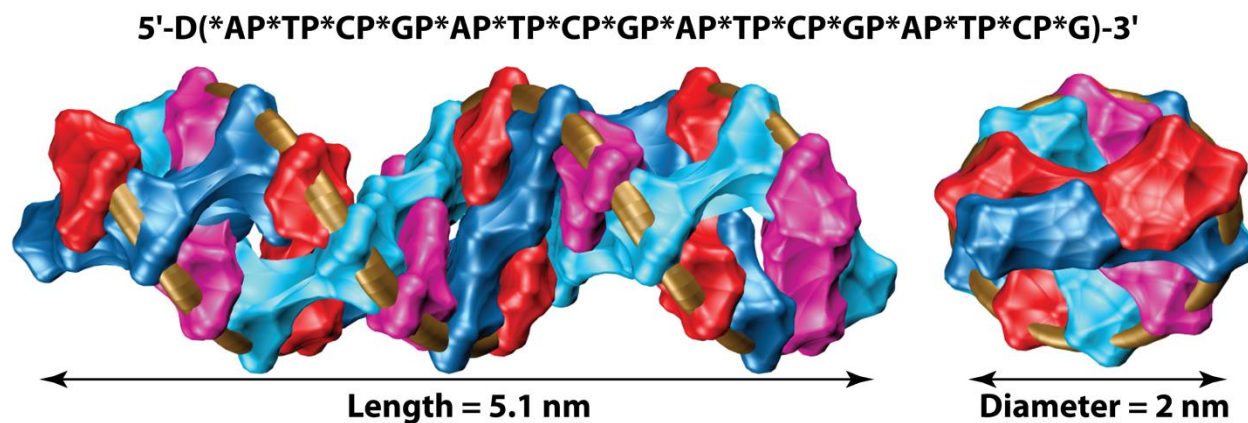


*Partial Denaturation of Double-Stranded DNA on  
Pristine Graphene under Physiological-Like  
Conditions*

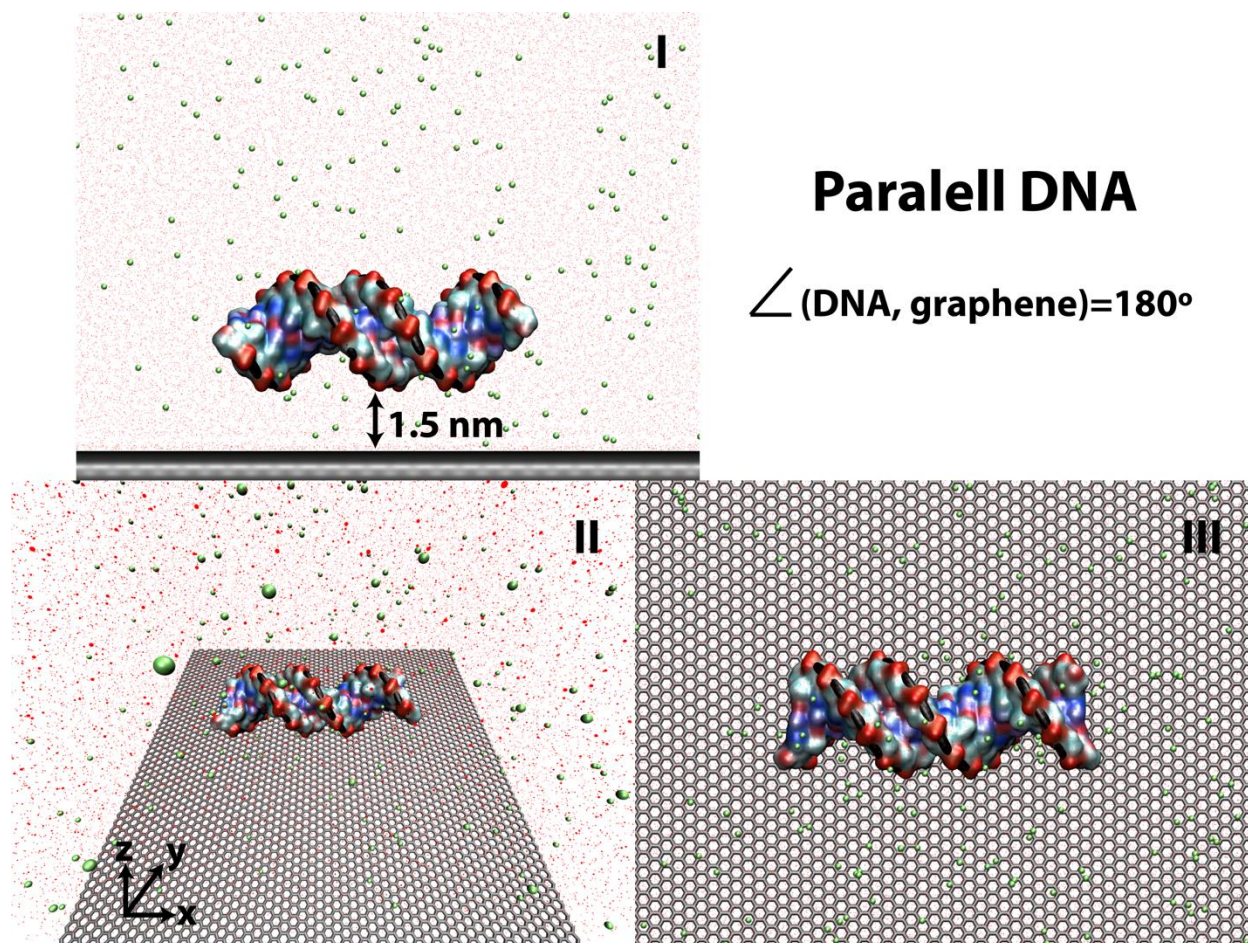
*Fernando J.A.L. Cruz\* and José P.B. Mota*

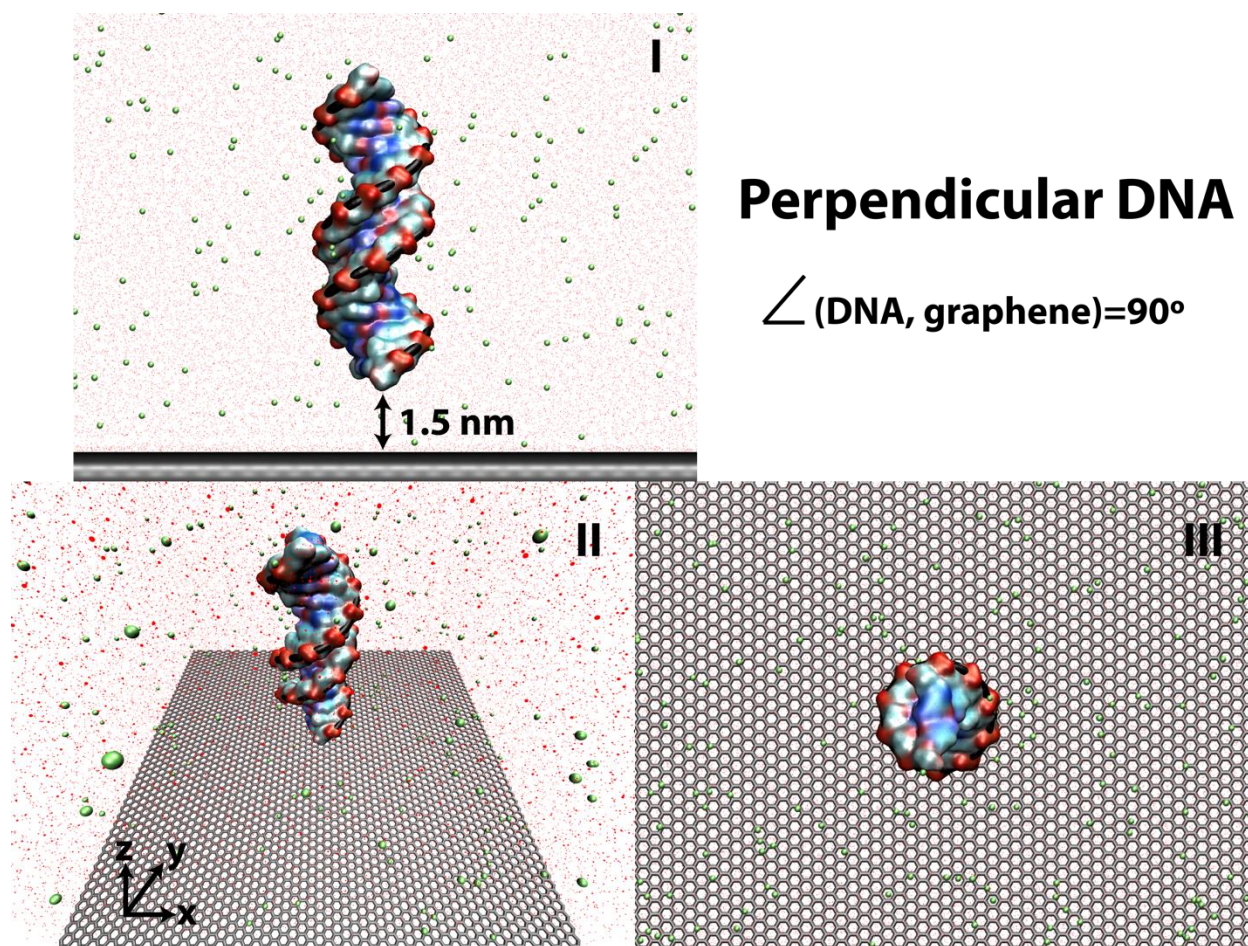
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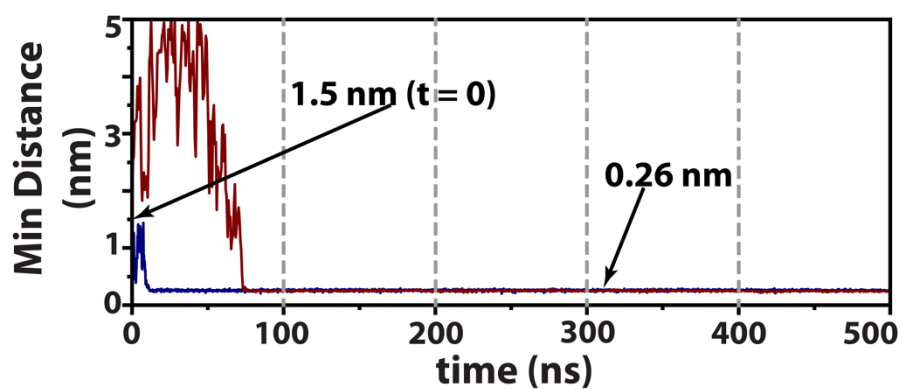


**Figure S1.** B-DNA hexadecamer (sequence: ATCGATCGATCGATCG). The nucleotides are coloured according to their individual nature, adenine (blue), thymine (red), guanine (magenta), and cytosine (cyan). The phosphate skeleton is depicted as a helical ochre line running through the double strand, with diameter 2 nm. The whole molecule is atomically detailed in the calculations.

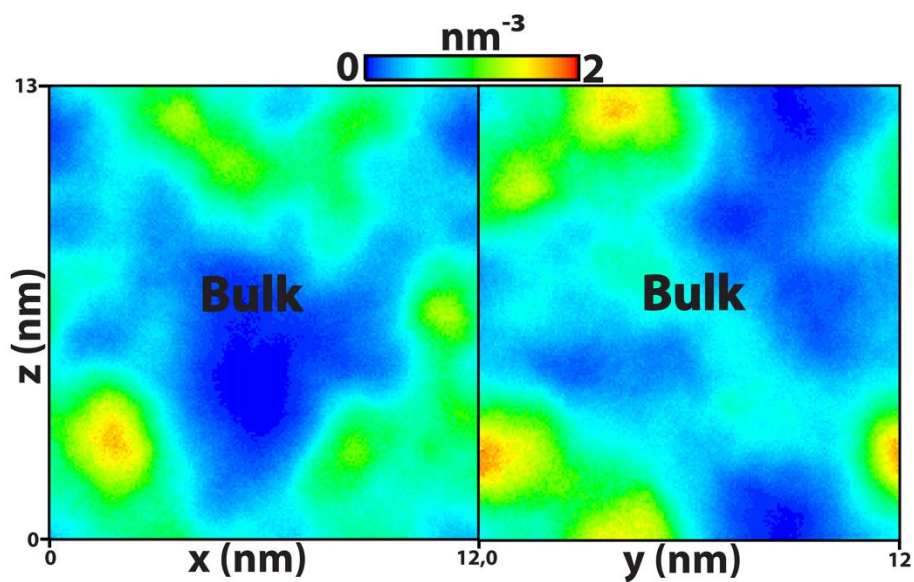




**Figure S2.** Initial system setup for parallel-oriented and perpendicular-oriented DNA. The  $sp^2$  carbon atoms are depicted as the characteristic honeycomb grey mesh representing the corresponding C–C bonds, and the DNA coloured according to the chemical nature of the individual nucleobases (N, blue; O, red; C, cyan) running through the phosphate skeleton depicted as a black cylinder.  $\text{H}_2\text{O}$  molecules are represented by red dots and both  $\text{Na}^+$  and  $\text{Cl}^-$  ions as green spheres.



**Figure S3.** Minimum distance between any DNA atom and the graphene surface. Parallel (blue) and perpendicular (dark red) configurations. Notice that the 0.26 nm plateau corresponds to direct contact between the nucleic acid and the graphene surface.



**Figure S4.** Two-dimensional number density maps of bulk DNA, obtained by histogram reweighting using a bin width of 0.07 nm.