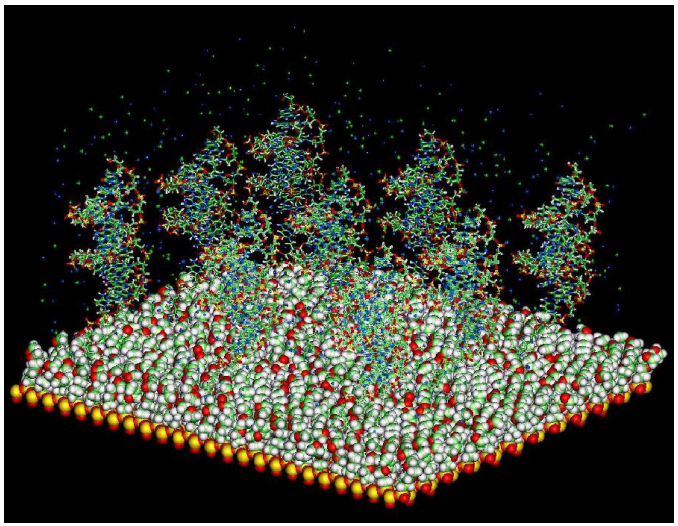
GC-7 Highlight

U. Houston

Muilti Scale Simulations in Biology and Chemisry



Simulation of DNA in saline solution on a prepared glass surface.

DNA microarrays, devices made of oligonucleotides tethered to surfaces, have recently had an explosion of interest. Fueled by advanced fabrication and signal detection techniques, their applications have reached diverse areas such as genetic screening/sequencing drug discovery and DNA computing. The DNA acts as a nano scale component in a micron scale detector. However, very little is known about the structure and physical behavior of the DNAs and their interactions when on the microarray surfaces. In order to understand the structure of the DNAs and their interactions when on the microarray surfaces, we performed the first all-atom molecular dynamics simulation of a DNA microarray. On the surface, the binding of the DNA is enhanced. The DNA duplex spontaneously tilted towards its nearest neighbor and settled in a leaning position. This close packing of the DNAs affects both in situ synthesis and deposition of probes on microarray surfaces.

"Spontaneous Formation of Structures on the Surface of DNA microarrays by an All-atom Molecular Dynamics Simulation" Theo. Chem. Accounts (2001); Ka-Yiu Wong and B.M.Pettitt.

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