SCIENCE SPRING DAY

FACULDADE DE CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA

Requimte/CQFB, Department of Chemistry

Nanothermodynamics of DNA Strands

UNIVERSIDADE NOVA DE LISBOA — OMNIS CIVITAS CONTRA SE DIVISA NON STABIT

requimte

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Dr. Cruz obtained his PhD in Chemistry at IST (Lisbon, 2006) and did a post-doc at Imperial College London (2006-2008). He has a track record of 15 peer-reviewed papers and 1 invited paper, and has been a referee for international journals.

Objectives

The project addresses two distinct but complementary areas: physical-chemistry and chemical biology. **Deoxyribonucleic acid** (DNA) and **single-walled carbon nanotubes** (SWCNTs) are prototypical one-dimensional structures: the first in life sciences and the second one in nanotechnologies. Their interactions have been partially investigated, nonetheless, the molecular-level details remain rather obscure; previous theoretical and experimental work has focused almost exclusively on exoadsorption of DNA at the SWCNTs exterior, precluding endohedral confinement. It is the goal of the present project to specifically address this issue. SWCNTs have been proposed for intracellular penetration, delivery of biological payloads and nucleotide sequencing. Apart from the biological relevance, DNA molecules confined in nanoscopic geometries are of fundamental importance for polymer physics.

Methodology

The kinetics and energetic features of the physico-chemical phenomena are probed in real time using **Molecular Dynamics** (MD) and enhanced sampling techniques derived from statistical mechanics (**umbrella sampling**, **metadynamics**). A hierarchical methodology is employed to study the systems (DNA+SWCNT+H_2O+ions) and (DNA+bacteriophage+H_2O+ions), spanning different time (ns–μs) and length scales (nm–μm). The boundaries are: *I)* fully atomistically detailed SWCNT and Dickerson dodecamer, which is the system employed to study the **nanoscale confinement of DNA** onto nanoporous solids (Fig.1), and *II)* genomic length DNA (> 1 kbps, L~ μm), with a nucleobase detailed potential, mimicking the encapsulation mechanism of double-stranded DNA onto **viral bacteriophage capsids** (Fig.2). Two different diameter SWCNTs are used (3 − 4nm), with null and positive charge density.

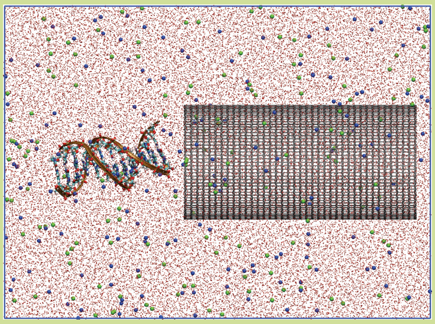

Fig.1 - Setup for the SWCNT studies. The system has orthorhombic symmetry and is surrounded by 3D periodic boundary conditions (blue lines). The double helix backbone is coloured ochre and the solid is represented as a grey mesh.

Na^+=blue spheres, Cl^-=green spheres and H_2O = red dots.

Expected Results

Ever since Watson and Crick unraveled the structure of the DNA double helix the latter has been considered as one of the building blocks of biological organisms. SWCNTs were first prepared in the 90s by Iijima and Bethune; numerous studies have helped to throw some light into the fascinating world of individual SWCNTs. The present project will make a significant and new contribution in the area of nanochemistry, bringing together in one physical system the bio (DNA) and nano building blocks (SWCNTs). At this level of complexity, scientists are still trying to answer some of the fundamentals: ***I)*** what is the influence exerted by the SWCNT upon the DNA thermodynamics?, ***II)*** is there a relationship between DNA sequence and configuration/mechanical properties upon confinement, ***III)*** is the encapsulation mechanism spontaneous?, ***IV)*** how fast is the latter?

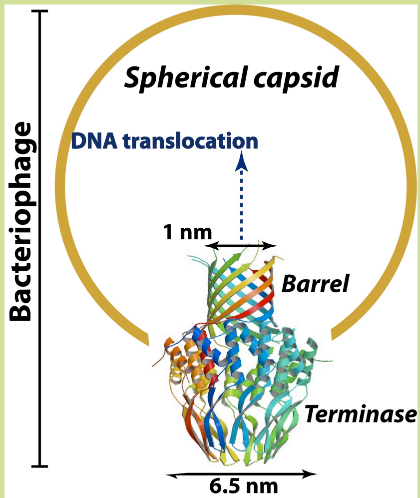

Fig.2 - Configurational diagram for the bacteriophage studies. The bacteriophage capsid is modelled with a spherical symmetry.

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