Modelling interaction of DNA with carbon nanostructures

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Abstract

This thesis focuses on the development of mathematical models for the interaction between deoxyribonucleic acid molecules (DNA) and certain carbon nanostructures. We model such atomic interactions by adopting the 6-12 Lennard-Jones potential and the continuum approach. The latter assumes that a discrete atomic structure can be replaced with an average constant atomic surface density of atoms that is assumed to be smeared over each molecule, in our case a DNA molecule and a carbon nanostructure. First, we develop a mathematical model for the interaction between a deoxyribonucleic acid molecule and a carbon nanotube, and we examine the storage of DNA molecules in carbon nanotubes. Following earlier authors, the carbon nanotube is modelled as a right circular cylinder, while the helical structure of the DNA molecule is modelled as a continuously twisted ribbon. We next determine the binding energies between DNA molecules interacting with a graphene sheet, and finally, we determine the binding energies of a C_{60} fullerene interacting with a DNA molecule.

Experiments in nanotechnology are often expensive and time consuming, and mathematical models and numerical simulations are necessary to complement the efforts of experimentalists and to confirm observed experimental outcomes. Despite recent improvements in the rapidity of numerical simulations, they can be more time consuming than the direct evaluation of an analytical expression arising from a mathematical model, because of the large numbers of atoms and force-field cal-

culations that may be involved. Although a mathematical model will necessarily include many assumptions and approximations, nevertheless often the main physical parameters and optimal configurations can be accurately predicted. The model calculations presented here for ideal systems, represent average outcomes, and generally there is good agreement with any existing numerical results that are obtained from more intensive computational schemes.

Here, we model the mechanics of the encapsulation of DNA molecules in carbon nanotubes to determine the optimal carbon nanotube that encloses the DNA molecule. The total interaction energy is calculated from the continuum approximation, where the atoms in each structure are assumed to be smeared over the surfaces of an ideal cylinder and a twisted ribbon, and the optimal carbon nanotube to enclose the DNA molecule is derived as the minimum energy configuration. Moreover, the binding energies between the DNA molecule adsorbing onto a graphene surface are derived by minimizing the binding energies to determine the preferred locations of the DNA molecules with respect to the graphene sheet. Finally, the binding of C_{60} to a DNA molecule is investigated, again by adopting the continuum approximation for modelling nanostructures.

In summary, the original contribution of this thesis is the development of ideal mathematical models and new analytical formulae for the interaction energy between deoxyribonucleic acid molecules and various types of carbon nanostructures, including carbon nanotubes, graphite, and C_{60} fullerene. The interaction energies between the DNA molecules and the nanostructures are determined analytically from the mathematical models and thus can be readily evaluated using standard computer algebra packages such as MAPLE and MATLAB. Hence, the interaction mechanisms and equilibrium configurations for a wide variety of systems might be fully and quickly investigated.

Signed Statement

I certify that this work contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution and, to the best of my knowledge and belief, contains no other material previously published or written by another person, except where due reference has been made in the text. In addition, I certify that no part of this work will, in the future, be used in a submission for any other degree or diploma in any university or other tertiary institution without the prior approval of the University of Adelaide. I give consent to this copy of my thesis when deposited in the University Library, being made available for loan and photocopying, subject to the provisions of the Copyright Act 1968. The author acknowledges that copyright of the published works contained within this thesis resides with the copyright holder(s) of those works.

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