Solving the Mystery of the Strikingly Different Mechanical Response of Nucleic Acids

The mechanical properties of nucleic acids (NAs) regulate multiple biological processes ranging from complex chromosome packing to replication of a plasmid. In vivo, NAs are not typically found in their relaxed forms. Instead, in the biological processes in which they take part, proteins wrap, bend, stretch, and twist double-stranded DNA (dsDNA) and double-stranded RNA (dsRNA) molecules. In spite of sharing a common double helix structure, single-molecule experiments have reported puzzling differences between their mechanical properties. dsRNA has a threefold softer stretching constant. More strikingly, dsDNA overwinds when stretched while dsRNA displays the expected unwinding response.

Understanding how a force induces changes in the structure of NAs at the atomic level is a challenge. In a recent publication in the Proceedings of the National Academy of Sciences (PNAS), researchers from the National Center for Biotechnology (CNB-CSIC) and from IFIMAC have used all-atom, microsecond-long molecular dynamics (MD) simulations to unveil the atomic-scale origin of the marked difference in the stretching response of dsRNA and dsDNA, their opposite twist-stretch coupling, and its nontrivial force dependence. They have implemented a new constant-force protocol, that closely mimics the single-molecule experiments, in order to simulate the structure of dsDNA and dsRNA subjected to stretching forces up to 20 pN. This methodology allows a direct determination of all of the elastic constants through the response of the average elongation, the average twist, and the coupling of their fluctuations to the applied force. A hierarchical analysis of these simulations sheds light into the physical mechanisms that control the mechanical response. The lower dsRNA stretching resistance is linked to its more open structure, whereas the opposite twist-stretch coupling of both molecules is due to the very different evolution of the molecules’ interstrand distance with the stretching force. A reduction of this distance leads to overwinding in dsDNA. In contrast, dsRNA is not able to reduce its interstrand distance and can only elongate by unwinding. The analysis of the parameters that characterize locally the double helix shows a direct correlation between the interstrand distance and the slide, the displacement of two consecutive base pairs in the plane perpendicular to the helical axis. In turn, the different behavior of the slide parameter of dsDNA and dsRNA can be traced down to the most fundamental difference between these two molecules: the extra hydroxyl group in the dsRNA sugar that connects the nitrogenous bases to the phosphate backbone. The comprehensive atomic-scale understanding of the mechanical response of NAs achieved in this study highlights MD simulations as a powerful tool to unveil the connection between forces and structure of NAs and, possibly, to gain insight into the associated changes in their biological functionality.

[Full article]

References
Condensed Matter Physics Center - IFIMAC through “Acreditación de Excelencia María de Maeztu” programme provides up to 4 Master Grants for candidates who wish to obtain an official master degree at Universidad Autónoma de Madrid related to IFIMAC. The call for proposal will be open from September 8th to September 22nd, 2017.
Deadline: September 22nd, 2017 at 15.00 h.
For more information please visit IFIMAC’s website.

Maxwell's Demon and Quantum Computers

INC COLLOQUIUM - OFFICIAL ANNOUNCEMENT
Title: Maxwell’s Demon and Quantum Computers.
When: 20 June, 2017, 12h30
Where: Sala de Conferencias, Módulo 00, Faculty of Science.
Speaker: Michel Devoret, Director of the Applied Physics Nanofabrication Lab, Yale University, USA.
ABSTRACT:

Can we prolong the coherence of a two-state manifold in a complex quantum system beyond the coherence of its longest-lived component? This question is the starting point in the construction of a scalable quantum computer. It translates in the
search for processes that operate as some sort of Maxwell’s demon, reliably correcting the errors resulting from the coupling between qubits and their environment. The presentation will review recent experiments that tested the dynamical protection, by Josephson circuits, of a logical qubit memory based on superpositions of particular coherent states of a superconducting resonator.

Complex Magnetic Structures at Surfaces and Their Imaging with STM from First Principles

Title: Complex Magnetic Structures at Surfaces and Their Imaging with STM from First Principles.
When: Monday, June 12, (2017), 12:00.
Place: Departamento de Física Teórica de la Materia Condensada, Facultad Ciencias, Module 5, Seminar Room (5th Floor).
Speaker: Krisztián Palotás, Department of Complex Physical Systems, Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia.

Recent advances in spin-polarized scanning tunneling microscopy (STM) experiments allow the determination of complex (non-collinear) surface magnetic structures (like spin-spirals, skyrmions) in real space. Motivated by these advancements, there is a strong need for theoretical understanding of the observed magnetic structures. In the first part of the talk I present recent theoretical results on the formation of a diversity of complex magnetic structures in thin films obtained by a combination of ab initio and spin dynamics calculations [1]. Understanding STM image contrasts is of crucial importance in surface science and related technologies. In the second part of the talk I present various STM theories and highlight different tip effects on the STM contrast based on first principles calculations, going beyond the Tersoff-Hamann model, e.g., within 3D-WKB tunneling theory [2]. Examples include a prototype frustrated hexagonal antiferromagnet, Cr monolayer on Ag(111) [3], metastable skyrmionic structures with various topologies [4] and highly oriented pyrolytic graphite. By comparing STM topographic data between experiment
and large scale simulations, we can determine particular tip orientations that are most/least likely present in the STM experiment [5]. Furthermore, I present an extension of Chen’s derivative rule for STM simulations including tip-orbital interference effects, and demonstrate the importance of such effects on the STM contrast for two surface structures: N-doped graphene and a magnetic Mn2H complex on the Ag(111) surface [6]. Finally, the first steps towards the theoretical modeling of high resolution spin transfer torque imaging are presented [7].

References
More information on IFIMAC Website