MARIE SKŁODOWSKA-CURIE INDIVIDUAL FELLOWSHIPS 2019

EXPRESSION OF INTEREST FOR HOSTING MARIE CURIE FELLOWS

HOST INSTITUTION

NOVA School of Science and Technology | LAQV – Associated Laboratory for Green Chemistry

RESEARCH GROUP AND URL

LATPE@Bio(chemical) Process Engineering
https://www.requimte.pt/laqv/index.php/research-groups/biochemical-process-engineering

SUPERVISOR (NAME AND E-MAIL)

Fernando J.A.L. Cruz
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SHORT CV OF THE SUPERVISOR

F. Cruz completed his PhD in Physical-Chemistry at Instituto Superior Técnico (Portugal, 2006), with a thesis entitled “Planetary Applications of Thermodynamics” under the supervision of Prof. Jorge Calado. He did a post-doc at Imperial College London (UK) from 2006 to 2008. Dr. Cruz has an h-index of 10 and a track record of 40 communications presented at international conferences, 23 papers published in international peer reviewed journals and 1 invited paper, almost all as first and/or corresponding author. He has been a referee for international journals (Carbon, PCCP, Nanoscale, Mol. Sim., J. Mater. Chem. B, J. Phys. Chem. B & C, Coll. Surf. A). F. Cruz was tutor of 3 PhD students (2006-2012, Portugal, UK), and has received grants from *Fundação Gulbenkian* and *Fundação para a Ciência e a Tecnologia* (Portugal), as well as from the *Engineering and Physical Sciences Research Council* (UK). At the present Dr. Cruz is a researcher at the host institution (LAQV@Requimte), working in the group of Prof. José Mota, and has been actively engaged in funded research projects at REQUIMTE (FCT Grants EXCL/QEQ-PRS/0308/2012, 2013-2015; PTDC/CTM/104782/2008, 2009-2012) and at Imperial College London (EPSRC Grant EP/ D035171/1, 2006-2008). F. Cruz has a proven track record of collaborative work and dissemination expertise, both inside the host institution and at the national and international level where he has been a visiting scholar at the Univ. Wisconsin-Madison (USA, 2010-11) and at the Ruhr-Universität Bochum (Germany, 2003).

5 SELECTED PUBLICATIONS

- F.J.A.L. Cruz and J.P.B. Mota, "Dynamics of B-DNA in Electrically Charged Solid Nanopores” *J. Phys. Chem. C* 121 (2017) 16568;
- F.J.A.L. Cruz, J.J. de Pablo and J.P.B. Mota, "Endohedral Confinement of a DNA Dodecamer onto Pristine Carbon Nanotubes and the Stability of the Canonical B Form", *J. Chem. Phys.* 140 (2014) 225103;
- F.J.A.L. Cruz and J.P.B. Mota, "Conformational Thermodynamics of DNA Strands in Hydrophilic Nanopores", *J. Phys. Chem. C* 120 (2016) 20357;

- F.J.A.L. Cruz and J.P.B. Mota, “Equilibrium and Transport Distributions of a DNA Dodecamer in Hydrophilic Nanopores”, *Materials Today: Proceedings* (2019) *in press*;

- F.J.A.L. Cruz, J.J. de Pablo, J.P.B. Mota, "Nanoscopic Characterization of DNA within Hydrophobic Pores: Thermodynamics and Kinetics ", *Biochem. Eng. J.* 104 (2015) 41.

PROJECT TITLE AND SHORT DESCRIPTION

Adsorption of DNA Strands onto 2D Surfaces

The sequence-dependent properties of DNA are critical for a several number of chemical and biological processes, however, few methods are able to probe them at the nucleobase/atomistic level. Classical experimental techniques in general yield only low-resolution information about shape, whilst others enlighten nothing about dynamics. A different approach is to study the phenomena occurring in real time, providing a self-consistent and simultaneous insight into thermodynamics and kinetics using Classical Molecular Dynamics coupled with enhanced sampling algorithms. We employ this powerful technique with an atomically-detailed descriptor of the whole system.

Here we propose to study the adsorption of short B-DNA strands onto 2D graphene surfaces, using theoretical-based approaches to probe the corresponding energetics and dynamics. Physiological conditions are employed, 310 K and [NaCl]=134 mM, allowing the direct extrapolation of results to biological phenomena of *in vivo* systems. Some of the questions to be answered are: *I)* what is the role played by the surface chemical functionality (*e.g.*, -NH2, -COOH, -CH3) and density? *II)* is there an optimal adsorptive state, regarding the geometrical biomolecule/solid orientation? *III)* what are the consequences upon the DNA hydrophilic and hydrophobic domains?

SCIENTIFIC AREA WHERE THE PROJECT FITS BEST

Chemistry (CHE) - Physical-chemistry