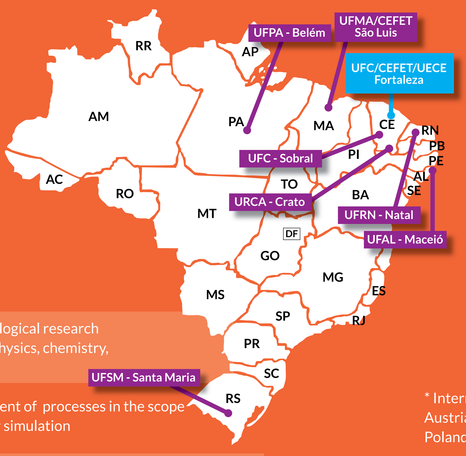
INCT NanoBioSimes

Coordinated and based on northeast 11 Institutions including universities and technological centers



General goals

Multidisciplinary view of the nanobiotechnological research subject, addressing knowledge frontiers in physics, chemistry, biochemistry, medicine and pharmacology

Technological applications and/or development of processes in the scope of nanobiostructures and nanobiomolecular simulation

Basic innovative research, which will offer new possibilities to be exploited in the field of nanoscience and nanotechnology

Inter-institutional collaborations already established in North and Northeast Brazil through previous networks

Research Topics

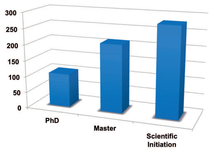
- Sensors
- Protein crystalization
- Pharmaceuticals
- DNA, RNA Transport properties
- Nanomaterials Nanotubes, Graphene, ...

* International collaboration with institutions in USA, France, Austria, Portugal, Belgium, Japan, Australia, German, UK, Poland, Argentina, Venezuela.

* Collaboration with INCT's Inomat e Nanocarbono

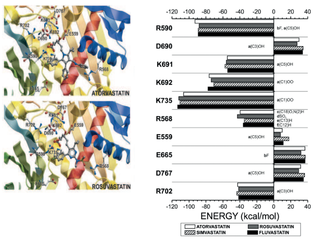
Scientific Production

- 817 Papers in refereed journals
- 28 Book Chapters
- 9 Patents



Pharmaceuticals Hot Paper (Royal Chemical Society)

A computational method to design drugs has been developed to design a new range of statins to lower cholesterol. Patents covering the leading statins have recently expired, including atorvastatin (Lipitor), with more to follow in 2012, so there is a pressure to develop new and more effective statin derivatives for the drug market. The new method involves using density functional theory to analyse the binding energies of new statins when they are bound to an enzyme involved in cholesterol biosynthesis.



R.F. da Costa et al, PCCP 14, 1389 (2012)

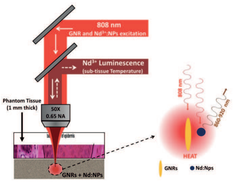
UFC-UFRN-IFCE Collaboration

Novel Nanothermometers and nanoheaters

(Rocha et al. ACS Nano, 2013, 7, 1188)

UFC-UFAL Collaboration

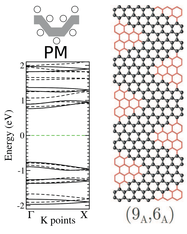
Schematic representation of the experimental setup used for single-beam sub-tissue-controlled hyperthermia. A 808 nm laser beam is focused into an aqueous solution containing gold nanorods (nanoheaters) and Nd3+:LaF3 nanoparticles (nanothermometers). The solution was placed under a 1 mm thick phantom tissue. Diagram at the right reflects the fact that both gold nanorods and Nd3+:LaF3 NPs were simultaneously excited by the 808 nm radiation.



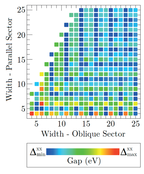
Novel graphene nanostructures

Girao et al., Phys. Rev. Letters 107, 135501 (2011).

This paper describes the electronic, optical and magnetic properties of novel carbon nanostrcutures (carbon nanowiggles).



Gap versus Geometry



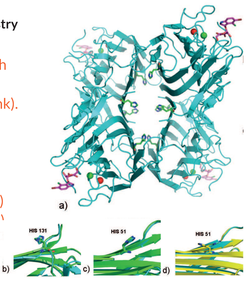
$\Delta^{AA}_{min} = 1$ meV, $\Delta^{AA}_{max} = 1.7$ eV

UFC-UFPB Collaboration

Protein crystallization

Bezerra et al. The International Journal of Biochemistry & Cell Biology 45, 807 (2013)

Overall structure of the lectin of D. violacea with the presence of Mn2+ and Ca2+ (red and green spheres, respectively) and the ligand X-Man (pink). This is an a plant lectin with vasorelaxant effects.The residues His51 and His131 are involved in oligomeric stablization. (b) Superposition of His131 in DVL (blue) and the lectin from Dioclea grandiflora (DGL) (green). (c) Superposition of DVL (blue) and DGL (green); (d) Lectin from D. guianensis (Dgui) (yellow) showing differences in the orientation of His51.

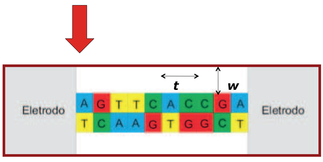


DNA Transport

L.M. Bezerril, et al, Appl. Phys. Lett. 98, 053702 (2011)

E.L. Albuquerque et al., Phys. Rep. in press.

UFC-UFRN-IFCE Collaboration



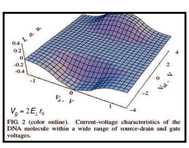


FIG. 2. (color online). Current-voltage characteristics of the DNA molecule within a wide range of source-drain and gate voltages.

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