CRETE CENTER FOR QUANTUM COMPLEXITY AND NANOTECHNOLOGY

ΣΕΜΙΝΑΡΙΟ ΚΕΝΤΡΟΥ ΚΒΑΝΤΙΚΗΣ ΠΟΛΥΠΛΟΚΟΤΗΤΑΣ & ΝΑΝΟΤΕΧΝΟΛΟΓΙΑΣ / CCQCN SEMINAR

Tuesday, 15 October 2013

11:00-12:00

3rd Floor Seminar Room

"Ab initio simulations of shock waves in biological media"

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&
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Abstract

Ion-beam therapy is a promising technique to destroy cancerous cells and tumors, in general. However, the detailed mechanism of how high-energy ions induce cell death is far from being well understood. It is generally accepted that the most effective way of killing cancerous cells is to arrest the cell cycle by inhibiting the reproductive ability of nuclear DNA. The main effect at MeV energies is to ionize the medium producing low-energy secondary electrons and radicals. In addition, the ionization of molecules in the vicinity of the ion track brings the biological system out of equilibrium, exhibiting forces that drive a radial shock wave (SW) in the medium, where the molecules move at supersonic velocity. The energy carried by the SW is then distributed around the system, and can produce lesions to functionally important structures such as DNA, proteins or membranes. Here we explore the effect of these SW using *ab initio* molecular dynamics simulations. We have investigated the interaction of supersonic SW with a solvated nucleotide, and found that the SW causes bond breaking (usually the phosphodiester C-O bond linking the phosphate with the sugar) in the studied nucleotide, but only for high velocities. The mechanism is complex and further simulations are needed to extract reliable statistics. Nevertheless these simulations represent a first fundamental step to understand whether the SW are relevant or not, the kind of damage they produce in solvated biomolecules, and how they do it.

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