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Nanoscale materials (nanocomposites, nanowires, carbon nanotubes): Computational modelling and applications in molecular, cell biology and nanomedicine

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Discovering of carbon nanotubes (CNTs), by S. Iijima, [1] in 1991 was a revolution in nanoscience. (CNTs) possess extraordinary physico-mechanical properties, and could be used as reinforcement for nanocomposites (a matrix- polymer, ceramic etc. reinforced by CNTs). The aim of the work, presented could be formulated as follows: to give some basic studies, regarding to the mechanical behaviour of nanocomposites, and to discuss computational modeling of their properties. Nanowires, as nanoscale materials also have very important applications, as field effect transistor (NWFET), for example [2]. Also, some computational models, based on the classical mechanics theories and nanoparticles applications for cancer has been developed. Nanotechnology, based on gold nanoparticles (nanoshells, nanorods, nanotubes), and models for describing of their optical properties has been presented, [3,4]. Numerical algorithms and numerical author's FORTRAN programs have been proposed in the work. Numerical (computational) results for accounting for the effects parameters and classical model, has been obtained. Comparison between numerical results, obtained and experiments in literature shows a very good agreement. Applications of nanotubes, nanowires, nanorods, nanoparticles, nanodots, nanocomposites in molecular and cellular biology, medicine (nanomedicine) have been commented as well.



Figure. Applications of nanotubes, nanoparticles, nanocomposites etc. in technique, engineering, industry, molecular and cell biology, biomedical, medicine etc.

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