Challenges and Perspectives in Modelling Nanomaterials

Douglas S. Galvão

Applied Physics Department, State University of Campinas, Campinas-SP, Brazil

With the advent of Nanotechnology there is a renewed interestin developing new computational techniques, at different levels ofaccuracy (from atomistic to mesoscale),to model nanomaterials.This renewed interest is motivated, in part, by the growing demand onminiaturisation, new functionalities, and less power consuming systems.When the size scale is reduced, the existence of a free surface modifiessignificantly the dynamical aspects, in special with relation tostructural stability and cost of defect formation.In this presentation we will discuss the use of theoretical toolsto investigate some of these problems. In particular we willdiscuss unusual mechanical properties of carbon-based materialsat nanoscale (negative Poisson´s ratio [1]), how to exploit theseproperties to create functional macromaterials (artificial muscles fromcarbon nanotube yarns [2]), and the spontaneous formation of ´exotic´ complexmetallic structures (such as, suspended atomic chains and hollow silvernanotubes) that can exist only at nanoscale [3,4].

[1] L. J. Hall, V. R. Coluci, D. S. Galvão, M. E. Kozlov, M. Zhang, S. O. Dantas, and R. H. Baughman, Science v320, 504 (2008).

[2] M. D. Lima et al., Science v338, 928 (2012).

[3] M. J. Lagos, F. Sato, J. Bettini, V. Rodrigues, D. S. Galvão, and D. Ugarte, NatureNanotechnology v4, 149 (2009).

[4] L. D. Machado, S. B. Legoas, J. S. Soares, N. Shadmi, A. Jorio, E. Joselevich, and D. S. Galvão, Phys. Rev. Lett. v110, 105502 (2013)