

CARBON NANOSCROLLS: A NOVEL ELECTRO-MECHANIC ACTUATOR

Riccardo Rurali¹, Vitor R. Coluci² and Douglas S. Galvão²

¹*Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona,
08193 Bellaterra, Spain*

²*Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas,
CP 6165, 13083-970 Campinas, SP, Brazil*

Riccardo.Rurali@uab.es

We present density-functional calculations of the electronic structure and the electro-mechanical response of carbon nanoscrolls (CNSs) [1,2]. One of the most promising properties that CNSs exhibit is the ability to be radially flexible. This has important consequences for doping and chemical storage, but it is also a potential source for a giant electro-mechanical effect [1,3].

Our calculations show that though having similar properties to carbon nanotube for what concerns the axial sensitivity [4,5], CNSs exhibit a radial response upon charge injection which is up to one order of magnitude larger. Hence, CNSs provide a route to efficient electro-mechanical actuators for future molecular electronics applications.

In the low-injection charge regime a subtle interplay between population/depletion of the antibonding/bonding orbital and Coulomb forces determines the behavior of the CNSs, while in the high-injection charge regime the CNSs always expand due to Coulomb repulsion.

Like in graphene sheets, the electronic structure around Fermi energy is determined by the boundary electronic states. On the other hand, the electro-mechanical response originates in the central region of the wrapped sheet, where extra charge accumulates.

References:

- [1] S. F. Braga, V. R. Coluci, S. B. Legoas, R. Giro, D. S. Galvao, and R. H. Baughman, *Nano Letters*, **4** (2004) 881.
- [2] L. M. Viculis, J. J. Mack, and R. B. Kaner, *Science*, **299** (2003) 1361.
- [3] R. H. Baughman, C. Cui, A. A. Zakhidov, Z. Iqbal, J. N. Barisci, G. M. Spinks, G. G. Wallace, A. Massoldi, D. De Rossi, A. G. Rinzler, O. Jaschinski, S. Roth, and S. Kertesz, *Science*, **284** (1999) 1340.
- [4] Yu. N. Gartstein, A. A. Zakhidov, and R. H. Baughman, *Physical Review Letters*, **89** (2002) 045503.
- [5] M. Verissimo-Alves, B. Koiller, H. Chacham, and R. B. Capaz, *Physical Review B*, **67** (2003) 161401.

Figures:

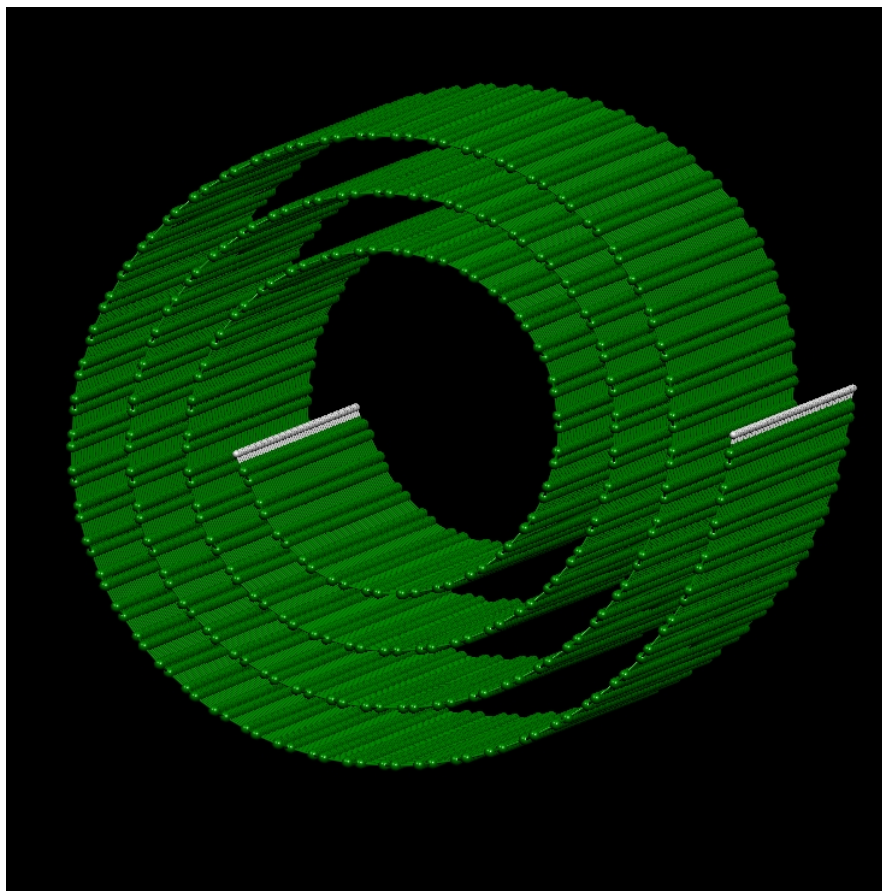


Figure 1 Snapshot of a CNS consisting of a jelly roll-like wrapping of a graphite sheet (with armchair profile, in the present case).