Twists and Turns in Nanocarbon Materials Modelling

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The anisotropy of low dimensional carbon nanoobjects such as graphene opens up possibilities for structural distortion modes and behavior not available to three-dimensional crystals. This talk explores the structure of edge dislocations in layered materials, using a combination of DFT and related tools with experimental support. Different dislocation orientation results in families of radically different structure types which exploit the available out-of-plane dimension [1,2]. Folding creates distinct Raman spectroscopic signatures [3] and can lead to local band gap variation in layered materials such as boron nitride [4].

The resulting low-symmetry folded, rolled, distorted and rippled sheets are interesting, not only in themselves, but also for the void spaces they create. There are a number of ways carbon can be used to confine other materials, either modifying bulk behavior or inducing unique low-dimensional change in the materials they are hosting [5]. Examples include the formation of new 1D material phases of intercalants such as phosphorus [6]. Via a combination of theory and experiment, we show that encapsulation within intermediate diameter cavities (1.5-2.5 nm) results in red phosphorus-like chain formation, and from this are able to build up a low-dimensional phase diagram for phosphorus constrained in carbon cavities.

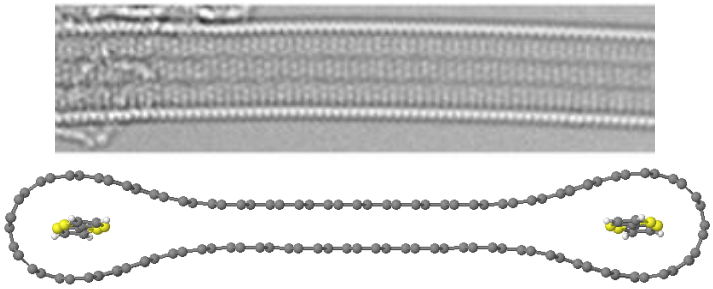

Figure 1. (top) Experimental image of phosphorus filled single walled carbon nanotube (bottom) collapsed carbon nanotube with filling of the edge cavities.

Keywords: Carbon, DFT, Defects, dislocations, structure.

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