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Nano-prisons for atoms: Using carbon nanostructures for sequestration, storage, and selective materials synthesis

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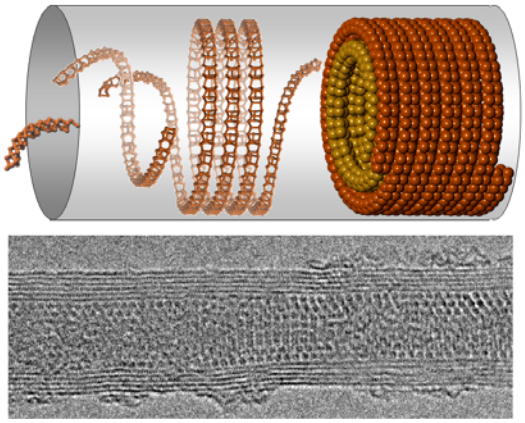

Figure 1. Top: Proposed formation mechanism of a helical phosohorus coil (Ref. [4]). Bottom: TEM micrograph of the coil embedded in a nanotube.(Ref. [5]).

Nanostrucutres consisting of graphitic carbon, including fullerenes, nanotubes and schwarzites, share the same high chemical, thermal and structural stability as wel as mechanical strength with monolayers of graphite. Chemically inert fullerenes and open-ended carbon nanotubes often benefit energetically by being filled with different atoms and molecules. Within the nanometer-wide cylindrical void, fullerenes may fuse to a nanotube [1], functionalized adamantanes and diamantanes fuse to carbon chains [2] or diamond nanowires [3]. Constraining molecules to a quasi-1D space may improve the selectivity of specific reactions including conversion of red phosphorus to helical coils [4,5], as seen in Fig. 1. The constrained volume inside the nanotube favors formation of previously unknown allotropes including Se helices [6] and metallic sulfur chains [7]. Schwarzites may be viewed as graphitic foams that fill rigidly 3D space [8,9] and may find similar uses as fullerenes and nanotubes, ranging from sequestration to selective formation of new materials. Computer simulations are a welcome means to gain microscopic insight into the physical properties and possible ways to synthesize these structures, as a guide to experimental efforts.

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