

From Nano-Prisons to Nano-Reactors: Using Carbon Nanostructures for Sequestration and Selective Materials Synthesis

David Tománek

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA • tomanek@pa.msu.edu

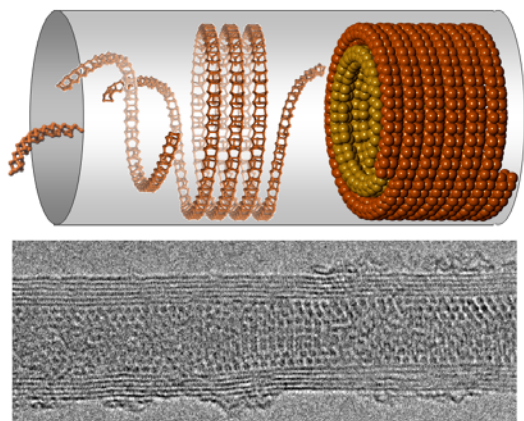


Figure 1. Top: Proposed formation mechanism of a helical phosphorus coil (Ref. [4]). Bottom: TEM micrograph of the coil embedded in a nanotube. (Ref. [5]).

Nanostructures consisting of graphitic carbon, including fullerenes, nanotubes and schwarzites, share the same high chemical, thermal and structural stability as well 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.

- [1] Seungwu Han, Mina Yoon, Savas Berber, Noah Park, Eiji Osawa, Jisoon Ihm, and David Tománek, [Phys. Rev. B **70**, 113402 \(2004\)](#).
- [2] Jinying Zhang, Yanquan Feng, Hitoshi Ishiwata, Yasumitsu Miyata, Ryo Kitaura, Jeremy E. P. Dahl, Robert M. K. Carlson, Hisanori Shinohara, and David Tománek, [ACS Nano **6**, 8674 \(2012\)](#).
- [3] Jinying Zhang, Zhen Zhu, Yanquan Feng, Hitoshi Ishiwata, Yasumitsu Miyata, Ryo Kitaura, Jeremy E. P. Dahl, Robert M. K. Carlson, Natalie A. Fokina, Peter R. Schreiner, David Tománek, and Hisanori Shinohara, [Angew. Chem. Int. Ed. **52**, 3717 \(2013\)](#).
- [4] Dan Liu, Jie Guan, Jingwei Jiang, and David Tománek, [Nano Lett. **16**, 7865 \(2016\)](#).
- [5] Jinying Zhang *et al.* [Angew. Chem. Int. Ed. **56**, 1850-1854 \(2017\)](#).
- [6] Toshihiko Fujimori, Renato Batista dos Santos, Takuya Hayashi, Morinobu Endo, Katsumi Kaneko, and David Tománek, [ACS Nano **7**, 5607 \(2013\)](#).
- [7] Toshihiko Fujimori, Aarón Morelos-Gómez, Zhen Zhu, Hiroyuki Muramatsu, Ryusuke Futamura, Koki Urita, Mauricio Terrones, Takuya Hayashi, Morinobu Endo, Sang Young Hong, Young Chul Choi, David Tománek and Katsumi Kaneko, [Nature Commun. **4**, 2162 \(2013\)](#).
- [8] Sora Park, Kritsada Kittimanapun, Jeung-Sun Ahn, Young-Kyun Kwon and David Tománek, [J. Phys.: Cond. Mat. **22**, 334220 \(2010\)](#).
- [9] Zhen Zhu and David Tománek, [Phys. Rev. Lett. **109**, 135501 \(2012\)](#).