*Colloquium talk at the Department of Physics, University of Science and Technology of China (USTC), Hefei, China, June 27, 2017*

# Nanoelectronics: From carbon nanostructures to 1D and 2D semiconductors beyond graphene*

David Tománek

*Physics and Astronomy Department, Michigan State University, East Lansing, MI 48824, USA*
tomanek@pa.msu.edu ● http://www.pa.msu.edu/people/tomanek

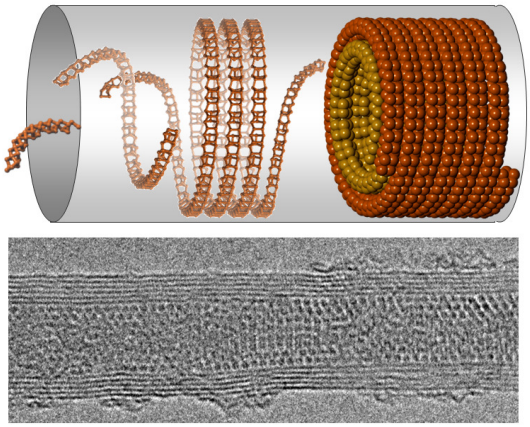

*Figure 1. Top: Proposed formation mechanism of a helical phosohorus coil (Ref. [7]). Bottom: TEM micrograph of the coil embedded in a nanotube.(Ref. [8]).*

If graphene had a band gap, it would probably be the optimum 2D system for electronics applications. Layered transition metal dichalcogenides (TMDs) with a robust intrinsic band gap appear as the next-best alternative. Only after a long search, however, optimum strategies have been devised to make low-resistance, ohmic contacts to TMDs [1]. In the meantime, a new class of 2D semiconductors has been rapidly gaining attention, namely layered black phosphorus and related phosphorene monolayers [2]. These 2D systems display a tunable, direct fundamental band gap and thus are ideal candidates for optoelectronics applications. Recent Quantum Monte Carlo (QMC) calculations show that the inter-layer bonding, while weak, is not well described by dispersive van der Waals (vdW) interactions [3]. QMC results differ qualitatively from vdW-enhanced DFT functionals and the common designation of similar systems as "van der Waals solids" is strictly incorrect. Also other group V systems including monolayers of $As_xP_{1-x}$ [4], IV-VI compounds such as SiS [5] with the same average valence, and related 2D phosphorus carbide [6] share the same nonplanarity of their structure with phosphorene. Same as in phosphorene, the fundamental band gap in these systems depends sensitively on the number of layers and in-layer strain. Surprisingly, the story of group V semiconductors does not end with layered 2D systems. A previously unknown 1D structure of coiled phosphorus, shown in Fig. 1, represents the most stable P allotrope to date. The predicted structure [7] has recently been synthesized and contained inside carbon nanotubes [8]. In all cases, predictive *ab initio* calculations provide a useful guidance to experimental studies.

* Partly supported by the NSF/AFOSR EFRI 2-DARE grant number #EFMA-1433459.

**References:**

[1] Jie Guan, Hsun-Jen Chuang, Zhixian Zhou, and David Tománek, ACS Nano **11,** 3904 (2017).
[2] H. Liu *et al.* *ACS Nano* **8,** 4033 (2014).
[3] L. Shulenburger, A.D. Baczewski, Z. Zhu, J. Guan, and D. Tománek, Nano Lett. **15**, 8170 (2015).
[4] Zhen Zhu, Jie Guan, and David Tománek, Nano Lett. **15**, 6042 (2015).
[5] Zhen Zhu, Jie Guan, Dan Liu, and David Tománek, ACS Nano **9**, 8284 (2015).
[6] Jie Guan, Dan Liu, Zhen Zhu, and David Tománek, Nano Lett. **16**, 3247 (2016).
[7] Dan Liu, Jie Guan, Jingwei Jiang, and David Tománek, Nano Lett. **16**, 7865 (2016).
[8] Jinying Zhang *et al.* Angew. Chem. Int. Ed. **56**, 1850-1854 (2017).