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

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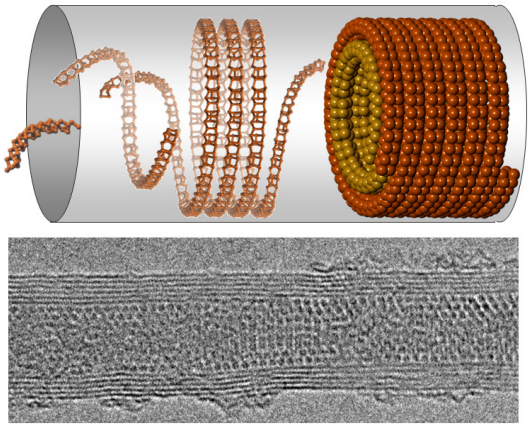

Figure 1. Top: Proposed formation mechanism of a helical phosohorus coil (Ref. [7]). Bottom: TEM micrograph of the coil/ring structure embedded in a nanotube (Ref. [8]).

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.

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References:

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