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### *Games that scientists play with carbon and phosphorus nanostructures*

Graphene monolayers, have sparked off unprecedented interest due to their unique electronic structure, but will unlikely replace silicon electronics due to a vanishing fundamental band gap. To still realize the promise of 2D semiconductor electronics, scientists are turning to other layered materials with a nonzero band gap. In this respect, layered structures of group V elements are rapidly attracting interest. Few-layer phosphorus dubbed phosphorene combines high carrier mobility with an unprecedented tunability of the band gap [1-3]. Multiple allotropes of phosphorene, illustrated in Figure 1, may be synthesized by CVD and coexist within a monolayer with virtually no energy penalty to form grain boundaries [4]. Similar to graphene, phosphorene may form fullerenes and nanotubes [5]. There are countless possibilities to tile a phosphorene monolayer with different allotropes, providing the possibility of complex electronic structure patterning [6]. Similar intriguing electronic properties as found in phosphorene are postulated also for arsenene, a monolayer of gray arsenic. 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.

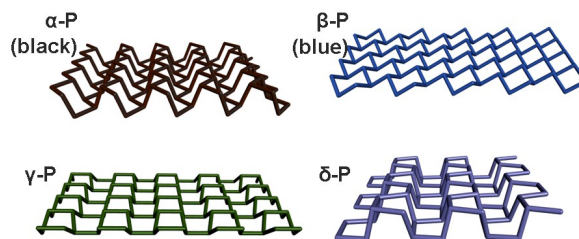


Figure 1. Different structural phases of phosphorene (Ref. [3])

- [1] David Tománek, 2014 symposium on phosphorene: An emerging 2D semiconductor, Mater. Express 4, 545 (2014).
- [2] Han Liu, Adam T. Neal, Zhen Zhu, Zhe Luo, Xianfan Xu, David Tománek, and Peide D. Ye, ACS Nano 8, 4033 (2014).
- [3] Zhen Zhu and David Tománek, Phys. Rev. Lett. 112, 176802 (2014).
- [4] Jie Guan, Zhen Zhu, and David Tománek, Phys. Rev. Lett. 113, 046804 (2014).
- [5] Jie Guan, Zhen Zhu, and David Tománek, Phys. Rev. Lett. 113, 226801 (2014).
- [6] Jie Guan, Zhen Zhu, and David Tománek, ACS Nano 8, 12763 (2014).

**David Tománek** studied Physics in Switzerland and received his Ph.D. from the Free University in Berlin. While holding a position as Assistant Professor of Physics in Berlin, he got engaged in theoretical research in Nanostructures at the AT&T Bell Laboratories and the University of California at Berkeley. He established the field of Computational Nanotechnology at Michigan State University, where he holds a position as Full Professor of Physics. His scientific expertise lies in the development and application of numerical techniques for structural, electronic and optical properties of surfaces, low-dimensional systems and nanostructures.

Since he was working on his PhD Thesis, he promoted the use of computer simulations to understand atomic-level processes at surfaces and in atomic clusters. Witnessed in several hundred publications and invited talks are his results on the electronic structure, mechanical, thermal, and optical properties, as well as quantum conductance of nanostructures. His contributions to Computational Nanotechnology, in particular in the field of fullerenes and nanotubes, have been rewarded by a Fellowship of the American Physical Society, the Alexander-von-Humboldt Foundation Distinguished Senior Scientist Award, the Japan Carbon Award for Life-Time Achievement, and the Lee Hsun award in Materials Science.

**Wednesday, December 2, 4:00 pm | 136 Jorgensen Hall**  
**3:45 pm – refreshments in Jorgensen Atrium**

Host:  
Professor Peter  
Dowben

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