

# Magic with Graphene and Phosphorene

David Tománek

Physics and Astronomy Dept., Michigan State University, East Lansing, MI 48824, USA  
[tomanek@pa.msu.edu](mailto:tomanek@pa.msu.edu)

Like in a magic trick, atomically thin layers of specific materials can be mixed and stacked in a well-defined way. Due to the inter-layer interaction and charge transfer, the heterostructure may exhibit unexpected behavior. In elemental boron, a previously unknown 2D  $\epsilon$ -B allotrope converts stepwise to a stable honeycomb structure when doped heavily with electrons, resembling a magic conversion of boron to carbon with one extra valence charge [1]. As seen in Fig. 1(b), this extra charge may be provided by an adjacent 2D  $\text{Ca}_2\text{N}$  electride layer. A different apparent example of magic involves the twist degree of freedom in 2D structures including bilayer graphene. Changing the twist angle  $\theta$  changes the Moiré pattern, as seen in the left panel of Fig. 1(c). Recent evidence suggests that the electronic structure near the Fermi level of twisted bilayer graphene (TBLG) depends extremely sensitively on the twist angle  $\theta$ . Near the magic angle value  $\theta_m \approx 1.08^\circ$ , a flat band emerges at  $E_F$ , separated from conduction and valence states by energy gaps, with important consequences for 2D superconductivity and electron correlation. Even though TBLG and related non-periodic structures can not be treated by standard band structure theory, their electronic structure can be interpreted quantitatively using a parameterized model [2] that can be simply extended to consider also other deformations including shear [3]. A third example of apparent magic involves a transformation of elemental phosphorus to unexpected nested coil structures when inside nanometer-wide carbon nanotubes [4,5].

This study was supported by the NSF/AFOSR EFRI 2-DARE grant number #EFMA-1433459.

## References

- [1] Dan Liu and David Tománek, *Effect of Net Charge on the Relative Stability of 2D Boron Allotropes*, [\*Nano Lett.\* \*\*19\*\*, 1359-1365 \(2019\)](#).
- [2] Xianqing Lin and David Tománek, *Minimum model for the electronic structure of twisted bilayer graphene and related structures*, [\*Phys. Rev. B.\* \*\*98\*\*, 081410\(R\) \(2018\)](#).
- [3] Xianqing Lin, Dan Liu and David Tománek, *Shear instability in twisted bilayer graphene*, [\*Phys. Rev. B.\* \*\*98\*\*, 195432 \(2018\)](#).
- [4] D. Liu, J. Guan, J. Jiang, and D. Tománek, *Unusually stable helical coil allotrope of phosphorus*, [\*Nano Lett.\* \*\*16\*\*, 7865 \(2016\)](#).
- [5] J. Zhang, D. Zhao, D. Xiao, C. Ma, H. Du, X. Li, L. Zhang, J. Huang, H. Huang, C.-L. Jia, D. Tománek, and C. Niu, *Assembly of Ring-shaped Phosphorus inside Carbon Nanotube Nanoreactors*, [\*Angew. Chem. Int. Ed.\* \*\*56\*\*, 1850-1854 \(2017\)](#).

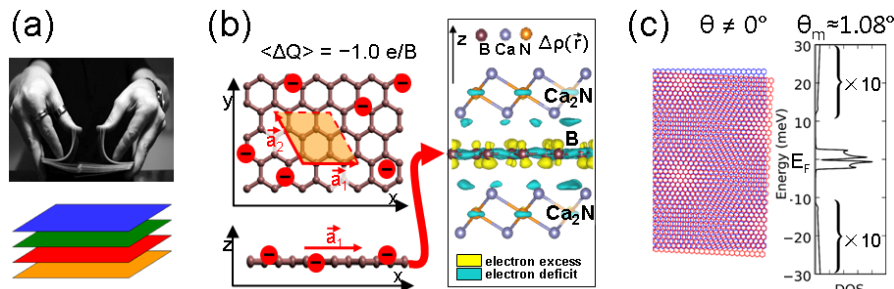


Figure 1: (a) Card magic illustrating the van der Waals assembly of 2D materials to a functional nanostructure. (b) Conversion of a 2D boron monolayer to a honeycomb lattice due to electron doping provided by a 2D electride. (c) Unusual changes in the electronic structure of twisted bilayer graphene near the magic twist angle  $\theta_m \approx 1.08^\circ$ .