Designing electronic properties of two-dimensional crystals through optimization of deformations

Vitor M. Pereira, Gareth W. Jones, Dario A. Bahamon

Graphene Research Centre & Department of Physics.
National University of Singapore, 2 Science Drive 3. Singapore.
vpereira@nus.edu.sg

Abstract

One of the enticing features common to most two-dimensional electronic systems that, in the wake of (and in parallel with) graphene, are currently at the forefront of materials science research is the ability to easily introduce a combination of planar deformations and bending in the system. Since the electronic properties are ultimately determined by the details of atomic orbital overlap, such mechanical manipulations translate into modified (or, at least, perturbed) electronic properties.

Graphene, in particular, on account of its exceptional range of elastic deformation, and peculiar electron-phonon coupling captured by the concept of a pseudo-magnetic field, has taught us that its intrinsic electronic properties can be molded by many more, and much richer, approaches that can be applied to 3D bulk solids. The ability to manipulate the local strain distribution in graphene opens the enticing prospect of strain-engineering its electronic and optical properties, as well as of enhancing interaction and correlation effects.

This presentation will beging with the introduction of examples of how strain-engineered graphene can have richer spectral, transport, and optical properties, and the presentation of a summary of recent experimental work exploring some of these new avenues.

At the core, a general-purpose optimization framework for tailoring physical properties of two-dimensional electronic systems by manipulating the state of local strain will be presented and discussed. This new framework allows a one-step route from the design of specific functionalities and device behavior to their experimental implementation.

As one example of its application, it will be shown how it efficiently answers the inverse problem of determining the optimal values of a set of external or control parameters (such as substrate topography, sample shape, load distribution, etc.) that result in a graphene deformation whose associated pseudomagnetic field profile best matches a prescribed target. Another example to be discussed is the typical problem of optimizing external parameters in order to make a graphene nanodevice perform with pre-defined target transport characteristics.

The ability to address this inverse problem in an expedited way is one key step for practical implementations of the concept of two-dimensional systems with electronic properties strain-engineered to order. This presentation will try to convey our approach to it.

References

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