Band Gap Opening in Graphene on Transition Metal Dichalcogenides and Related Substrates

J .R. Wallbank[1], M. Mucha-Kruczyński[1,2] and V. I. Fal'ko[1]

[1] *Department of Physics, Lancaster University, Lancaster, LA1 4YB, UK*
[2] *Department of Physics, University of Bath, Claverton Down, Bath, BA2 7AY, UK*

It is often be desirable to open a band gap in graphene for use in electronic devises, however many techniques that do so also result in a reduction of the carrier mobility. In contrast, placing graphene on atomically flat crystal substrates often results in a dramatic increase in carrier mobility. Furthermore, an exactly aligned hexagonal substrate with a lattice constant exactly $\sqrt{3}$ times bigger than that of graphene, would result in a Kekulé distortion, inducing intravalley mixing and band gap opening at the Dirac point. Indeed there are many substrates, including certain transition metal dichalcogenides, that almost fit the requirement. However a slightly deviation from the $\sqrt{3}$ times bigger lattice constant or any misalignment angle will result in the formation of the quasi-periodic structure known as a moiré pattern.

The dominant effect of the moiré on graphene electrons can be described in terms of scattering using the simplest moiré harmonics, which, when combined with the symmetry of the system, allows the Hamiltonian to be written in terms of a small number of phenomenological, substrate dependant, parameters [1]. Like the Kekulé distortion, but in contrast to the thoroughly investigated case of graphene on substrates with comparable lattice constants [1], the $\sqrt{3}$ times bigger substrates result in intervalley scattering, allowing new parametric regimes to be explored.

We investigate the characteristic features that appear in the resulting graphene moiré miniband spectrum, systematically exploring the space of phenomenological substrate parameters. We show that the Dirac spectrum around zero energy always remains intact, in contrast with the Kekulé distortion. However, for a large parametric regime, a band gap is still opened by these substrates, but between the first and second moiré minibands. The remaining possibilities being that either the first and second minibands do not touch, although overlap on the energy axis, or, will touch at six highly anisotropic mini Dirac points.

[1] J. R. Wallbank, A. A. Patel, M. Mucha-Kruczynski, A. K. Geim, V. I. Fal'ko, arXiv:1211.4711 (2012)