Graphene on Antidot Lattice

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Abstract

In recent years, graphene antidot lattices (GALs) have received great attention due to their ability to strongly alter the electronic properties of graphene, in some cases inducing a sizable electronic band gap [1]. Concurrently, bilayer graphene (BLG) has been studied as an alternative way of achieving semiconducting graphene-based structures, with a band gap tunable via an inter-layer bias [2]. While many studies have focused on combinations of pristine graphene and GAL structures, resulting in, e.g., GALbased waveguides [3], focus has so far been on structures retaining the single-layer nature of graphene. We propose instead a structure consisting of bilayer graphene, wherein one of the layers is periodically perforated, while the other one remains pristine, see Fig. 1. This results in a GAL vertically coupled to single-layered graphene (SLG), which we denote as GOAL (Graphene On Antidot Lattice).

Using a nearest-neighbor tight-binding calculations, we demonstrate that if the isolated GAL has a band gap, the resulting GOAL behaves as a hybrid between single-layer and bilayer graphene, with properties tunable via the gap of the GAL layer. In particular, in the absence of an inter-layer bias, the gap in the GAL layer forces the electrons to localize predominantly in the graphene layer, resulting in properties resembling single-layer graphene. However, we find that introducing a bias via shifted on-site energies results in a tunable band gap, similar to the case of BLG. The combined structure thus retains the linear bands of graphene in absence of bias, yet maintains a sizable and tunable band gap when an inter-layer bias is applied, see Fig. 2.

Using recursive Green's techniques we examine single-electron transport between semi-infinite BLG leads though a central GOAL region. We find that the device exhibits SLG-like transport within the gap of the GAL layer, albeit with slight modulations, including a non-zero transport at the Fermi energy, see the upper panel of Fig. 3. By expressing the bond currents in a recursive fashion similar to the recursive calculation of the transport coefficient, we are able to efficiently calculate the bond currents of large systems. These confirm that the current is restricted mostly to the graphene layer of GOAL as shown in the middle and lower panel of Fig. 3.

The linear bands at zero bias and sizeable gap at non-zero bias of GOAL suggests a powerful platform material for probing SLG-like properties. Unlike SLG, GOAL has the possibility to open and tune band gaps selectively throughout the material by appropriately applying inter-layer biasing.

References

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Fig. 2. The electronic band structure of PG (*gray*), GOAL with zero bias (*black*), and GOAL with non-zero bias (*red*). The GOAL materials have the triangular lattice GAL{7,3} [1]. These band structures are calculated from a TB model using BLG TB-parameters, only nearest neighbors, and uniform bias across all atoms with opposite signs in the two layers.



Fig. 3. Upper panel: The single electron transport pristine coefficient of graphene (black) and GOAL (red) between semi-infinite BLG leads. Both the leads and the device are periodic yielding an infinite 2D system. The GOAL has the lattice GAL{6,3} [1] and has a width allowing at least 9 lines of antidots. Also shown is the point-ofinterest for the bond calculation transport below. Middel and lower panel: The single electron transport bond currents throughtout the graphene layer (middel) and antidot layer (bottom). The currents are displayed by summing outgoing current vectors of each atom in every hexagon in the respective layers. Note that the current in the antidot layer is practically zero, hence no visible arrows.