Disorder-induced localised gating in graphene

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Disorder-induced localised gating in graphene

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Introduction
Gating of individual atoms in graphene would allow extremely precise control of current flow. In practice, however, this is very difficult to achieve. In this work we investigate whether doping or spatially restricted gating can be used to achieve similar control. Two systems are considered:

- Sublattice asymmetric doping within a region in a pristine graphene sheet [1,2].
- Sublattice symmetric gated region in a pristine graphene sheet [4].

Why Patched Green’s Functions?
When computing the effect of disorder, the main challenges are the “low” number of atoms that can be considered at once, and the corresponding boundary conditions, typically edges or periodicity. An alternative is to use the Patched Green’s Functions method [3], where the boundary conditions are replaced by a boundary selfenergy. This enables one to effectively imbide a region into a periodic material, as long as a simple expression for the real-space Green’s Functions is available.

Green’s Function of Graphene

The onsite potential is shifted in one of the sublattices, with an average change (keeping the shift times concentration constant) of: ε_G = ε_A = 0.1|c|, for a varying concentration of atoms (c = 1.0, 0.5, 0.2) within a circular region of radius 20nm. The positive energies are the most interesting.

- c = 1.0
- c = 0.5
- c = 0.2

Figure from [1], showing sublattice imbalance in experiments

Density of states (shaded region is the pristine version)

- Log(DOS)

Density of states comparable to pristine

- Log(DOS)

Sublattice asymmetric potential

The onsite potential is shifted in one of the sublattices, with an average change (keeping the shift times concentration constant) of: ε_G = 0.2|c|; ε_A = 0, for a varying concentration of A-atoms (c_A = 1.0, 0.5, 0.2) within a circular region of radius 20nm.

DOS comparable to pristine

- Log(DOS)

Sublattice symmetric potential

The onsite potential is shifted in both sublattices, with an average change (keeping the shift times concentration constant) of: ε_G = 0; ε_A = 0.1|c|, for a varying concentration of atoms (c = 1.0, 0.5, 0.2) within a circular region of radius 20nm. The positive energies are the most interesting - ε_A = 0.

Log(DOS)

- Log(DOS)

- Log(DOS)

Conclusions
- The key features of the DOS for the asymmetrically doped dot are largely independent of c_A.
- The key features of the DOS for the uniformly gated dot are very dependent on the concentration. The peaks associated with the vortex behavior get completely smeared out.

References

Methods
We use:
- A 1NN tight binding model.
- The Patched Green’s Functions (PGF) method [3]
- The PGF is explained in the right column.
- A simple onsite energy shift for dopants

Conclusions
- The key features of the DOS for the asymmetrically doped dot are largely independent of c_A.
- The key features of the DOS for the uniformly gated dot are very dependent on the concentration. The peaks associated with the vortex behavior get completely smeared out.

References