Electronic and Optical Properties of Graphene Antidot Lattices

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While pristine graphene has presented a wealth of intriguing electronic properties, the lack of a sizable band gap is a significant drawback for possible applications in the field of electronics. We have shown how a periodic modulation of a graphene sheet, in the form of a regular array of holes, introduces a band gap around the Fermi level, the size of which depends on the size and periodicity of the holes [1]. While we have originally focused on perforations as the source of the modulation, several experiments have presented alternate methods of realizing such graphene antidot lattices, such as e.g. patterned hydrogen adsorption [2]. The crucial ingredient is the breaking of the symmetry between the two sublattices of graphene.

We present results of band structure calculations using three computational methods of increasing complexity; (i) finite-element solutions of the Dirac equation (DE) with an infinite mass term in the location of the antidots, (ii) nearest-neighbor tight-binding (TB) calculations, and (iii) full-fledged density functional theory (DFT) calculations. We find good agreement between DFT and TB calculations, while the DE method consistently reports larger band gaps. The discrepancies of the DE results are linked to the lack of an adiabatic transition between the perfect graphene sheet and a graphene antidot lattice with vanishing hole radius [3]. A simple correction of the DE results leads to much better agreement between all three methods.

The lower conduction and upper valence band of graphene antidot lattices can be described qualitatively in a simple continuum model, by introducing a mass term in the Dirac equation of pristine graphene. We present closed-form expressions of the optical conductivity predicted from such a model [4] and compare with results obtained from atomistic modelling [5]. The model admits analytical solutions, also with a magnetic field perpendicular to the graphene plane. Using these analytical solutions, we present preliminary results on the influence of magnetic fields on the optical properties of gapped graphene, with an emphasis on the off-diagonal conductivity. We compare these results to calculations using a tight-binding model with a staggered potential, where the magnetic field is introduced via a Peierls substitution.

References

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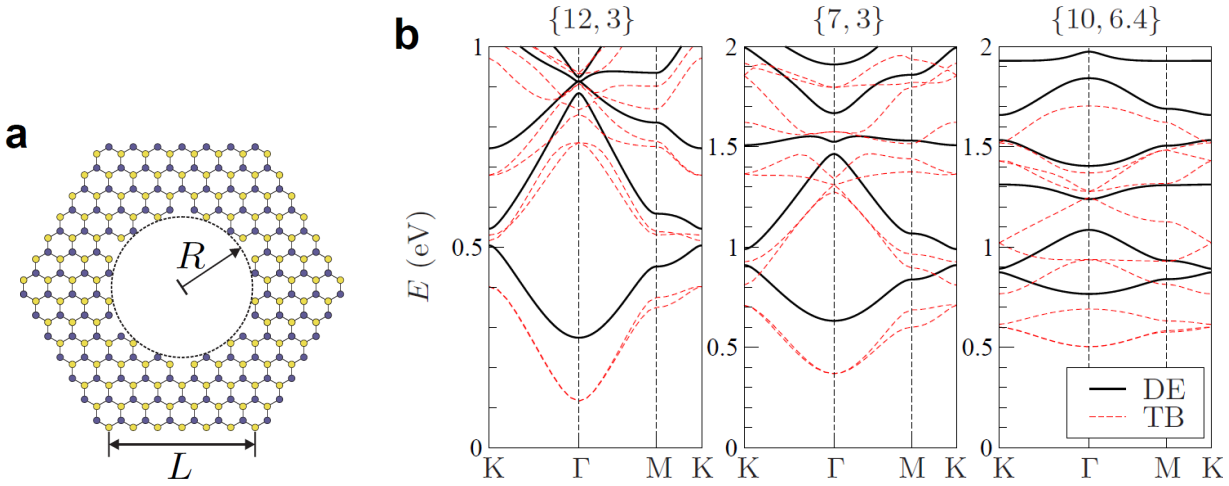
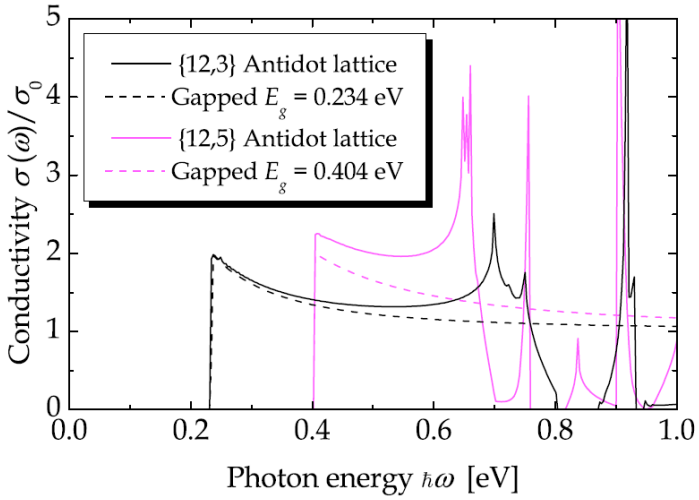
[2] R. Balog *et al.*, Nature Materials, **9** (2010) 315.
[3] J. Fürst *et al.*, New Journal of Physics, **11** (2009) 095020.
[4] T. G. Pedersen *et al.*, Physical Review B **79** (2009) 113406.
[5] T. G. Pedersen *et al.*, Physical Review B **77** (2008) 245431.

Figures



(a) Unit cell of the {L,R}={7,3} graphene antidot lattice, with L and R given in units of the graphene lattice constant. (b) Band structure calculated for three different antidot lattices, comparing results obtained using the Dirac equation to those obtained using a nearest-neighbor tight-binding approach. Only positive energies are shown, as both methods exhibit perfect electron-hole symmetry. Note that while the methods are in qualitative agreement on the shape of the bands, the DE results consistently show larger band gaps.



Optical conductivity calculated for gapped graphene compared to results obtained using atomistic modelling of graphene antidot lattices. The mass term of the gapped graphene has been adjusted to fit the band gap of the chosen antidot lattices. Note the qualitative agreement at low energies.