

# Graphene antidot lattices and barriers studied with the Dirac equation

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## Abstract

A band gap can be introduced in graphene by periodic nanoporation, called a graphene antidot lattice (GAL). This effect has been demonstrated both theoretically [1, 2] and experimentally [3, 4]. Several methods have been used to produce GALs experimentally, including e-beam lithography [3], diblock copolymer templates [4], barrier-guided growth [5], nanosphere lithography [6] and nanoimprint lithography [7]. The antidots range in size between a few nanometers and several hundred nanometers, depending on the fabrication method.

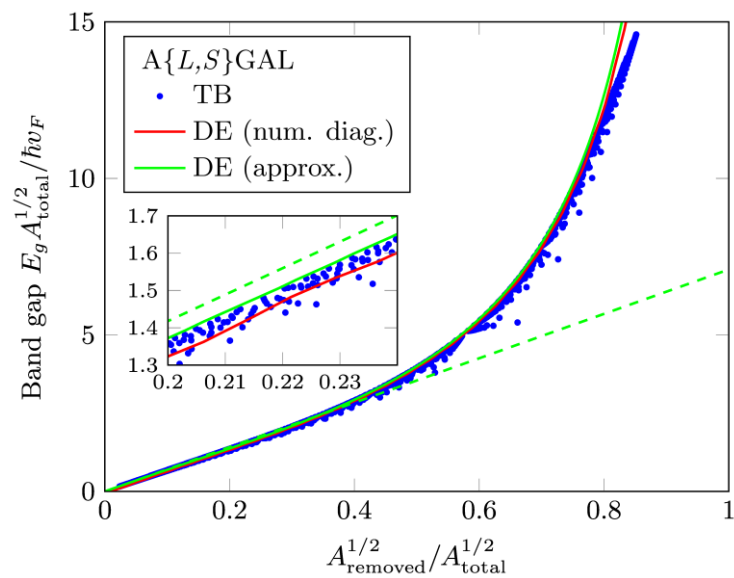
Experimentally feasible structures are typically much larger than what traditional theoretical methods, such as tight-binding (TB) or density functional theory, can handle. We present novel methods based on the Dirac equation (DE), which enables us to calculate properties of very large structures. In fact, there is no additional computational cost for increasing the size of the unit cell. We use a spatially varying mass term to model GALs, where the mass term is non-zero in the antidot regions and vanishing elsewhere [2]. The mass term effectively makes electrons massive inside the antidots, which makes it unfavorable to enter them.

First, we set up a model that enables us to calculate electronic and optical properties of fully periodic GALs. We compare the results of our models with TB and show excellent agreement in the case of antidots with armchair edges. Figure 1 shows a comparison of bands gap calculated using TB and our Dirac model. Next, we look at electronic transport in graphene antidot barriers (GABs). A GAB can be made by introducing a 1D GAL strip in an otherwise pristine sheet of graphene. We solve this as a scattering problem, where a plane electron wave is incident on a GAB. Using this method, we can calculate the resulting wave function as well as the conductance spectrum of the barrier. An example of the electron probability density of a barrier is shown for different energies in Figure 2. The conductance is high at an energy of 0.15 eV, which results in a high probability density inside the barrier, whereas a low conductance at 0.30 eV results in a low probability density.

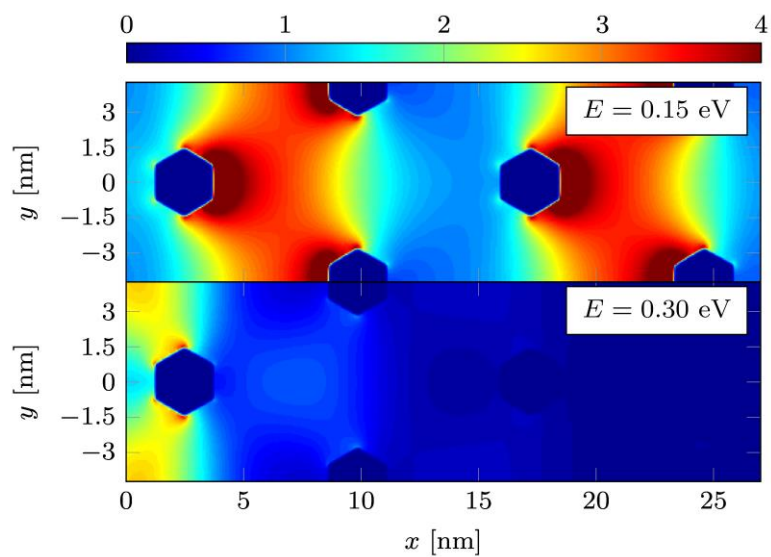
## References

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## Figures



**Figure 1.** Comparison of band gaps calculated using TB and the DE.



**Figure 2.** Electron probability density of a GAB with 4 hexagonal antidots.