Band Gap Engineering in Graphene Nanomeshes

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Abstract

Despite having an extremely high carrier mobility [1], the straightforward use of graphene in digital electronics industry is precluded, among other factors, by its semimetallic character. Thus, great efforts have been made in order to open a gap in graphene and render it a semiconductor. These include adding an extra dimension of confinement, obtaining graphene nanoribbons (GNRs) [2], electrostatic patterning [3], chemical decoration [4], etc.

Another possibility that has been reported in order to open a gap in graphene is the use of nanolithographic patterning to define an antidot lattice [5,6], also called a graphene nanomesh (GNM), where a periodic arrangement of (possibly passivated) holes is defined onto a graphene layer. We will present first-principles studies of the effect of hole shape, size, pitch, passivation and lattice type on the band structure of GNMs.

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References

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Figures

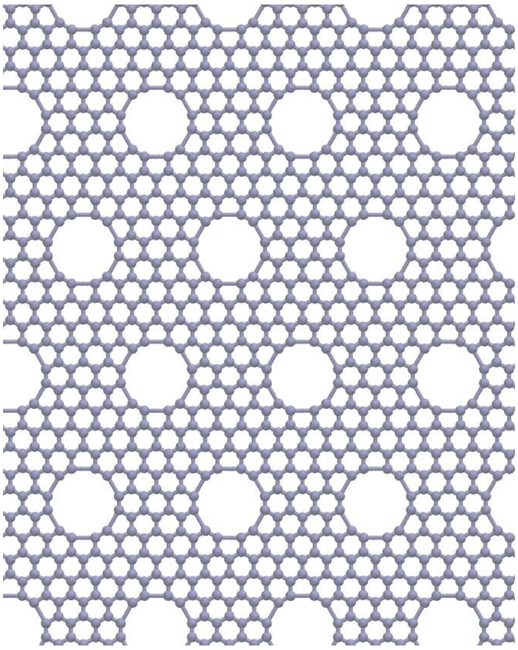

Fig. 1: Relaxed 6x6 graphene supercell with C_{12} holes (12 C atoms removed) in a hexagonal lattice arrangement.

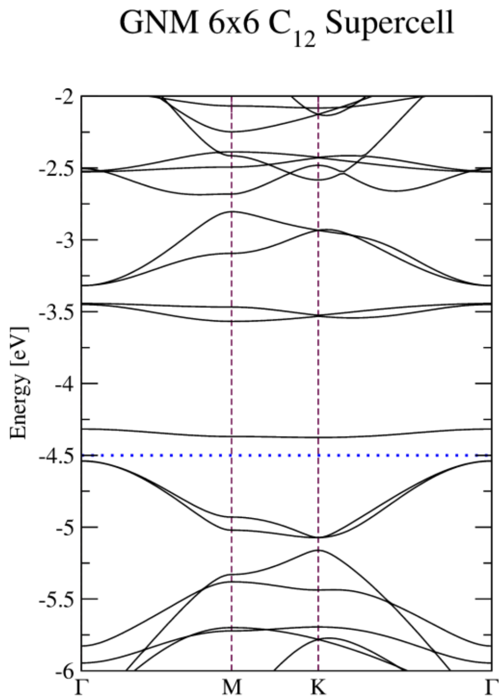

Fig. 2: Band diagram corresponding to the structure in Fig. 1. The band with low dispersion right above the Fermi level corresponds to hole edge states.

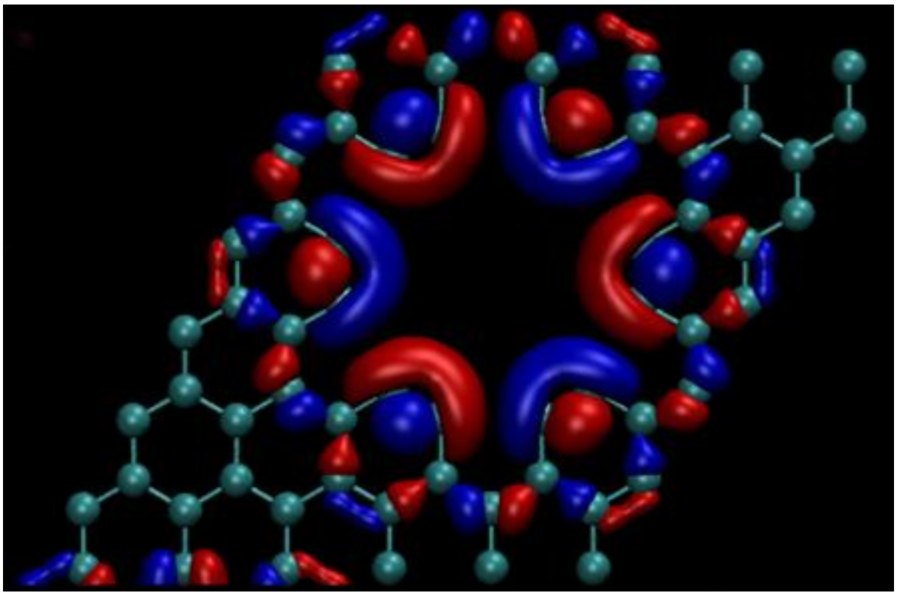

Fig. 3: Wavefunction isosurface plot for the LUMO in Fig. 2. Its low dispersion in the band diagram and the preferential localization of the wavefunction indicate that it is an edge state. Blue (red) indicates positive (negative) phase.