Stability of Dirac cone in artificial graphene

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What is the Artificial Graphene (AG) ?

It's an artificial material that exploits the properties of graphene in a tunable setup. Actually It has been realized 3 different physical implementations:
- 2D electron gas in a semiconductor heterostructures
- Metal surfaces shaped by molecules
- Trapped cold atoms in an optical lattice

Benefits of using AG:

- Great spatial accuracy to better control Dirac Fermions
- Lattice constants from tenths nm to hundreds nm
- Alternative texturing, like Kekulé distorsion

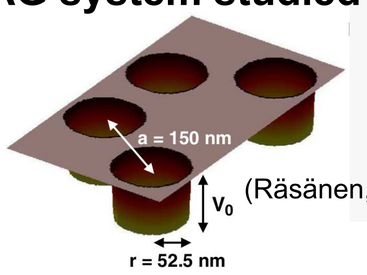
Previous works: for electrons confined in GaAs quantum dots:

- Tight binding calculations of Gilbertini et al.[1] show graphene-like bands;
- Confirmed by DFT results (Räsänen, Rozzi [2]).

Present work :Study of the stability of AG Dirac cone in GaAs QD with respect to changes in the following parameters:

- dots potential shape;
- dots potential radius;
- dislocations of atoms position;
- lattice constant change.

AG system studied

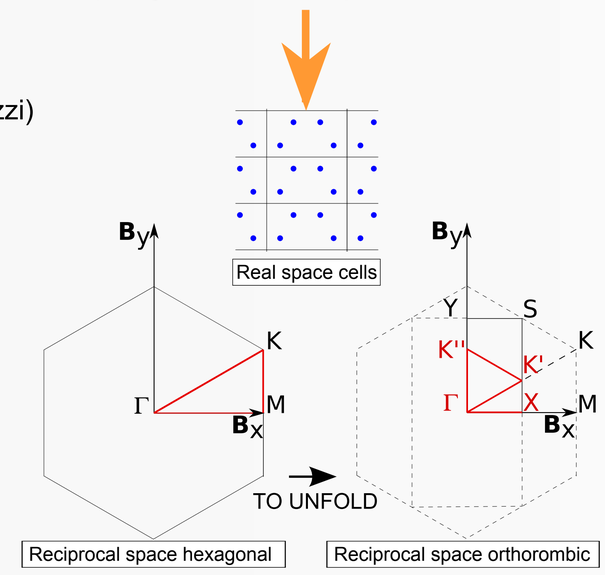


(Räsänen, Rozzi)

System details:
dot-dot distance = 150 nm.
N = 1 electron per dot.
Hard-wall potential (or exponential)
$v(x) = -V_0\ \Theta(|x-r|)$
Potential radius r = 52.5 nm
(hard-wall case).
Potential depth = V0 = -0.6 meV

For reproducing electrons in GaAs QD:
Electron effective mass m = 0.067
Dielectric constant ε = 12.4

Orthorombic supercell of 4 atoms: an unfolding procedure is required for comparing the ΓMKΓ band path.



Theory and computational method

2D system periodic in 2D.
Theory: independent particles (IP), DFT-LDA, DFT-mGGA
Bloch wavefunctions in real space (Octopus Code 4.0.1) [3]
Kohn-Sham equations with periodic boundary conditions.

Convergence parameters: - mesh spacing (0.2-0.3 effective bohr)
- number of k-points in the irreducible Brillouin zone (300-600).
Usage of Broyden mixing and symmetrization of the density.

LDA: Slater Exchange LDA (PAM Dirac) + AMGB correlation (Attaccalite) [4]
mGGA: exchange PRHG07 [5,6] + AMGB correlation (Attaccalite).

Change of potential shape and dot radius

A possible improvement of the forementioned model of electrons in GaAs dots, can be obtained by the replacement of the hard-wall potential with a more realistic one of exponential shape, i.e. :

Dot potential: $v_{dot}(r) = V_0 exp(-\frac{r}{L})^{\alpha}$

We performed IP, LDA and mGGA calculations varying the exponent α (=2,4,8,12) and the effective radius L from 0.1 to 0.5 times the dot-dot distance a (= 150 nm).

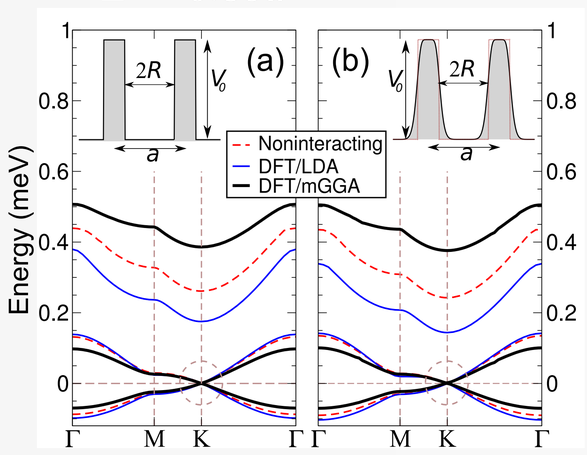
Results:

- Little change occurs varying α;
- There is an optimal window of L values that optimizes the stability for all the calculations ([0.30,0.40] times the dot-dot distance "a")

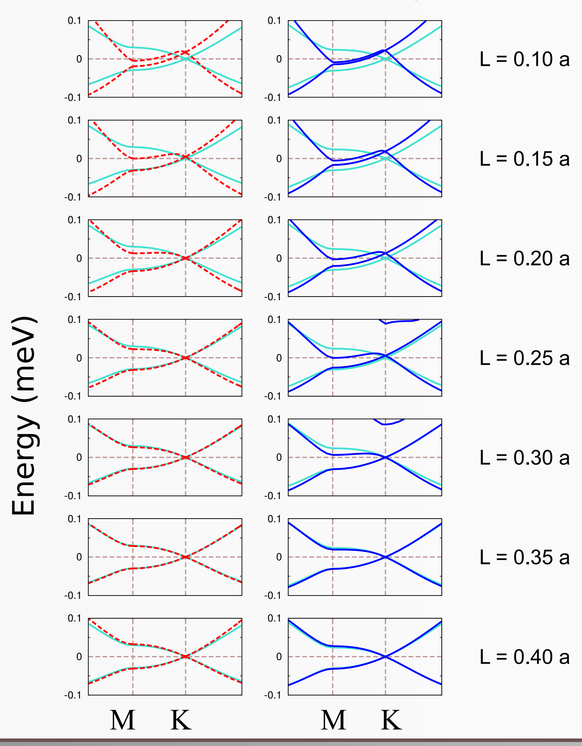
Parameters of maximal stability:

$\alpha = 8$

$L = 0.35a$



Optimal L window



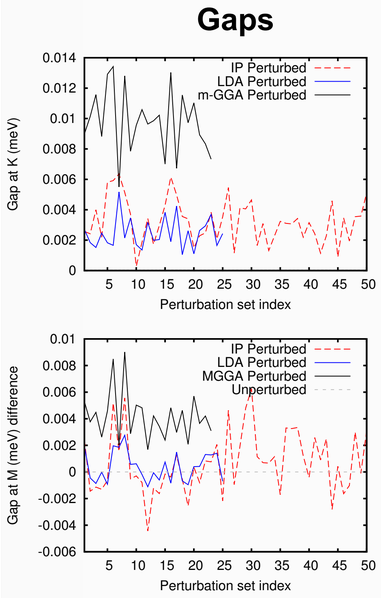
Dislocation of atoms position.

We applied to all the atoms of the cell a dislocation with modulus 0-%2 of the dot-dot distance and with random angle in [0,2 π].
- 50 random dislocation sets used for IP, 25 for LDA and 25 for mGGA.

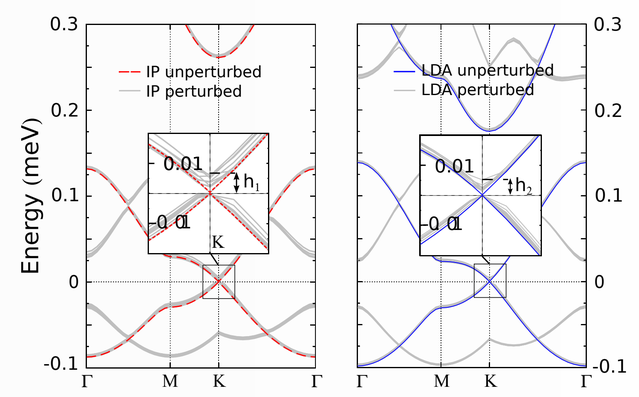
Results:

- There is always a gap opening but is always less than $1.4x10^{-2}$ meV.
- LDA shows the highest stability, DFT-mGGA is the less stable but its variation is of the same order of magnitude for the gaps at K and M and for the bands in general.
- The DOS mimum change is very small -> furher stability. -------

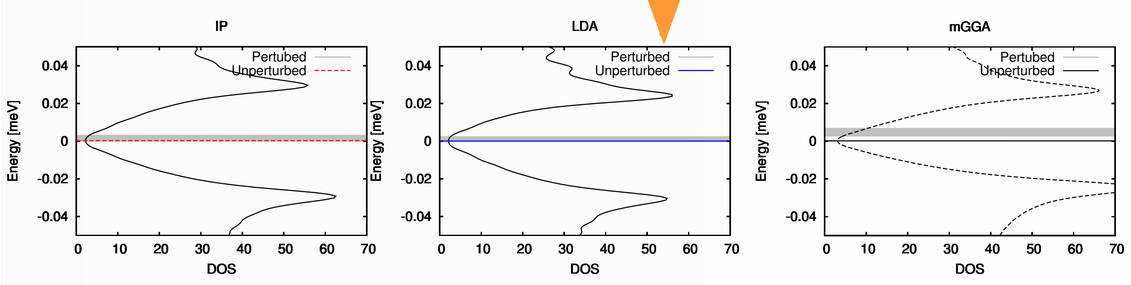
Gaps



All results overlapped



DOS minima

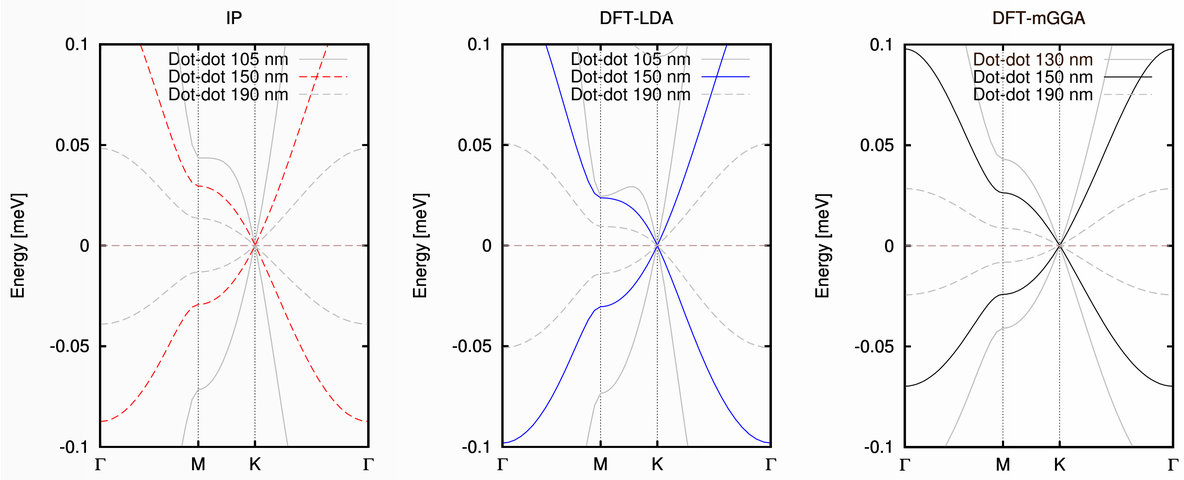


Change of lattice constant

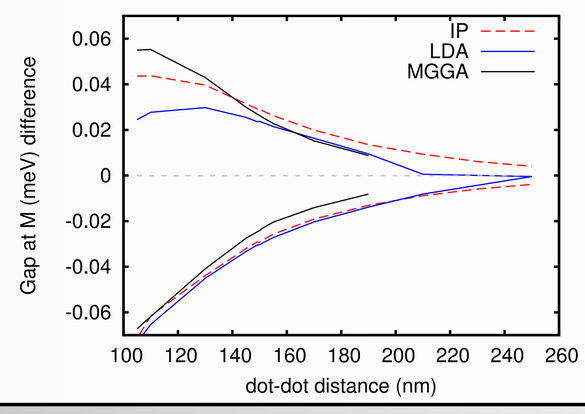
Dot-dot distance from 105 nm to 250 nm (till 190 for mGGA) and the Dirac cone is maintained.

Results:

- We can see that the system experiences a transition towards metallicity for an increasing dot-dot distance
- The process is faster in presence of e-e interaction than for IP calculation.



Gaps →



Future developments

- Spin polarized case
- Studying effect of repulsive potentials in triangular lattices instead of attractive potentials in honeycomb lattices
- Optical properties

Bilbiography

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