Study of magnetism induced by vacancies in graphene

Nanoelectronics

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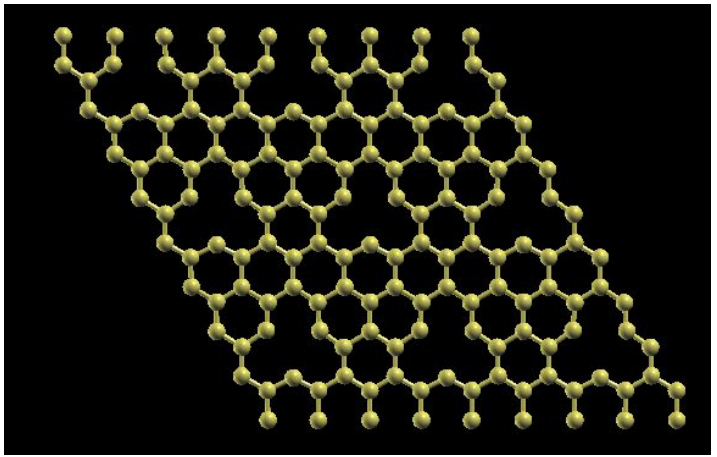
Introduction

- Spin-polarized density functional theory has been used to study the effects of vacancy defects on the magnetic properties of graphene sheet.
- Software: Quantum ESPRESSO, Xcrysden.
- Pseudopotential: PBE-GGA.
- Cell dimension: 7.4 x 7.4x 14.8 Å.



Workflow

Structural Optimization

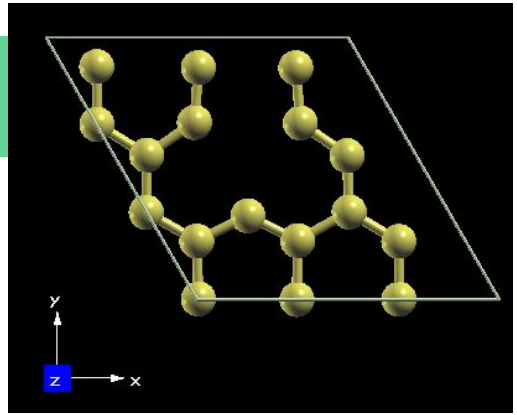
- Relax
- Convergence tests

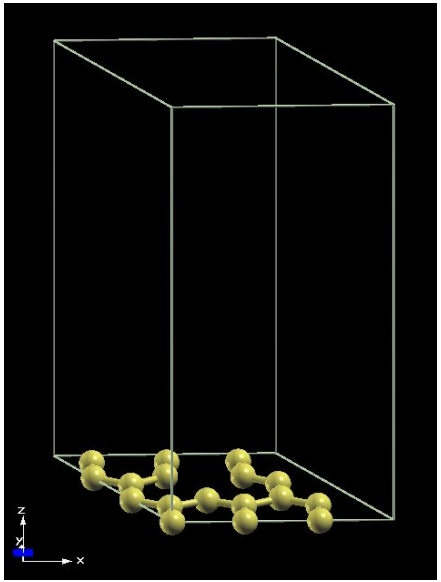
Calculation

- scf
- nscf

Post processing

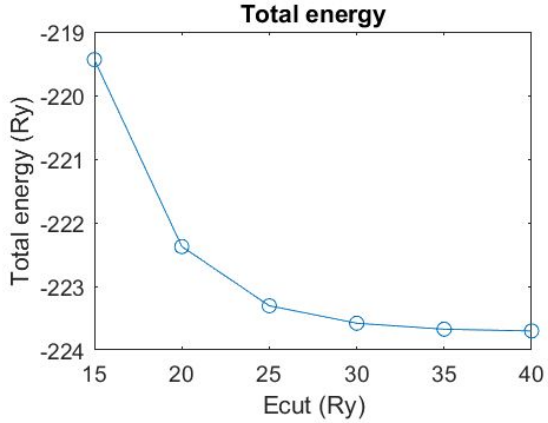
- DOS
- Charge density

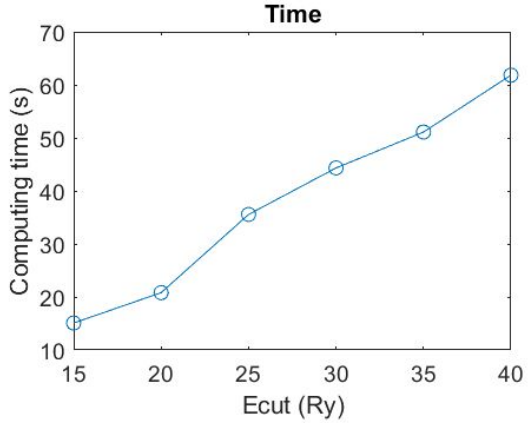


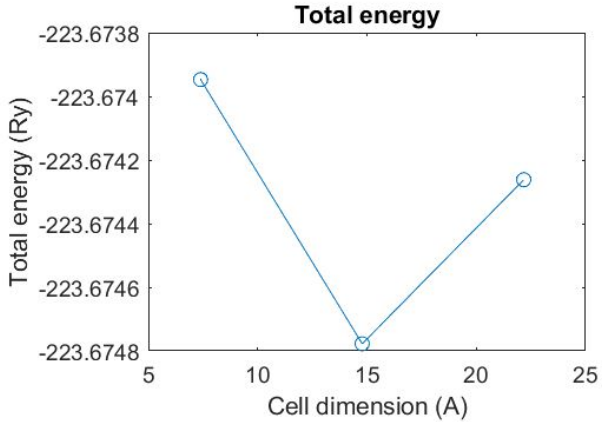


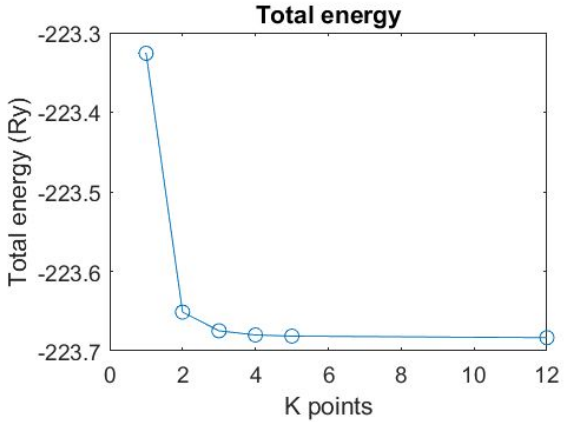
Graphene sheet input from http://www.fisica.uniud.it/~giannozz/QE-Tutorial/

Convergence tests









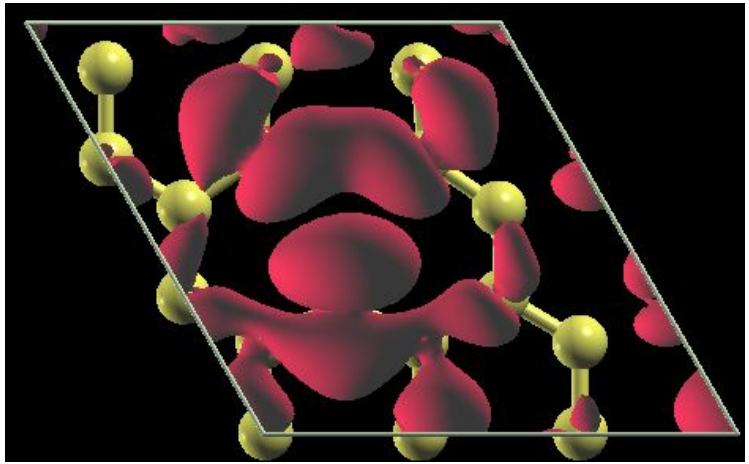
SCF calculation

```
          k = 0.3333 0.1925 0.0000 ( 16511 PWs)   bands (ev):

   -21.1806 -20.2927 -19.5865 -19.0569 -17.9490 -17.5579 -16.6139 -16.3579
   -15.1970 -14.0578 -13.7250 -13.4418 -12.5823 -11.2939 -11.2390 -10.8096
    -9.7143  -9.3084  -9.1447  -9.0739  -8.7627  -8.3218  -8.1061  -7.6678
    -7.2632  -7.0715  -6.7676  -6.7030  -5.4364  -5.1448  -4.8170  -4.4327
    -3.7888  -2.2224  -1.6924  -0.7614  -0.1340   0.2788   0.9683   1.5091
     1.5658

     the Fermi energy is    -2.2198 ev

!    total energy              =    -210.65619456 Ry
     estimated scf accuracy    <          5.4E-09 Ry
     smearing contrib. (-TS)   =      -0.00355933 Ry
     internal energy E=F+TS    =    -210.65263523 Ry

     The total energy is F=E-TS. E is the sum of the following terms:
     one-electron contribution =   -1251.04175879 Ry
     hartree contribution      =     637.28621081 Ry
     xc contribution           =     -78.39125975 Ry
     ewald contribution        =     481.49417250 Ry

     total magnetization       =       0.93 Bohr mag/cell
     absolute magnetization    =       1.24 Bohr mag/cell

     convergence has been achieved in  22 iterations
```

Magnetic moment results in the range 1.12-1.53 μ **B** , it depends on the number of atoms for cells and the number of vacancies.

Electronic and structural distortions

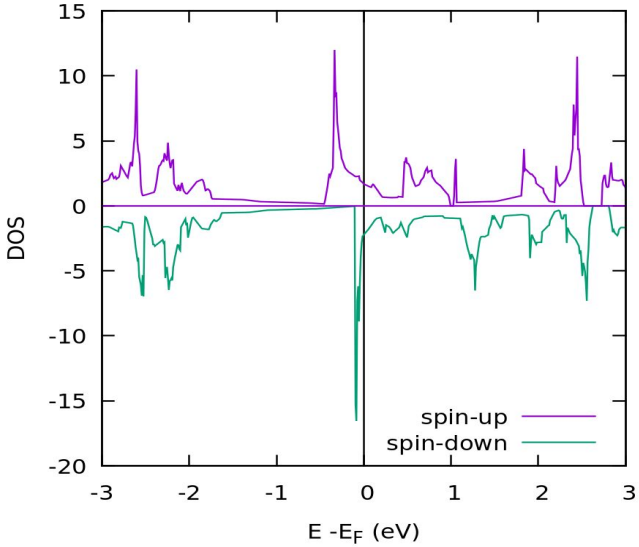
- Because of vacancy, it is broken three bonds sp^2.
- The structure experiences a distortion that leads to the saturation of two of the three dangling bonds toward the missing atom (Jahn-Teller distortion).
- The vacancy appears as a protrusion in STM images.
- In figure LDOS at the dangling bonds, obtained from DFT calculation.

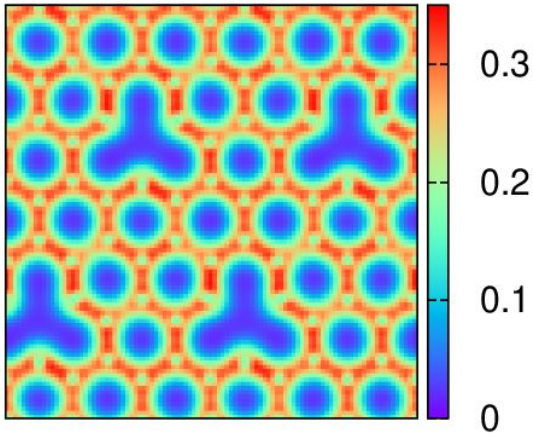


Isovalue: 0.0007

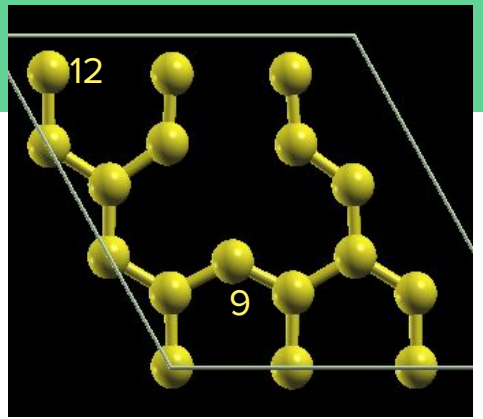
DOS

- The density of states of graphene with one vacancy is asymmetric. Thus, it is possible to deduce that graphene presents spin polarization.
- Single vacancy induces new states at Fermi energy.
- The figure below represents the total charge density.

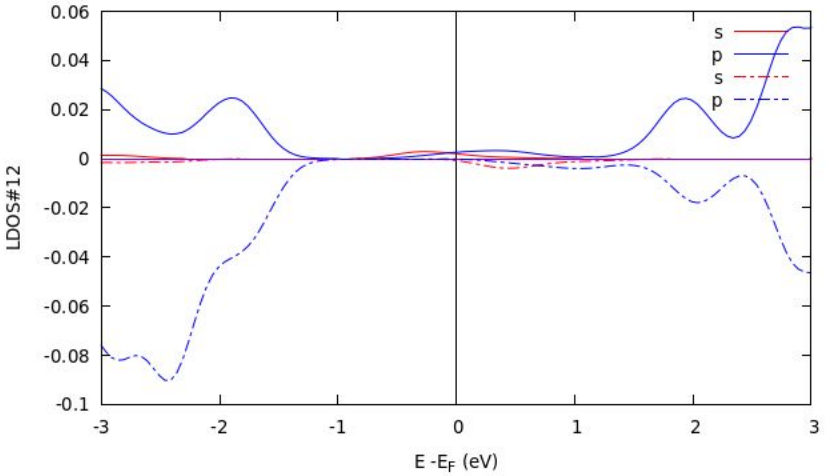


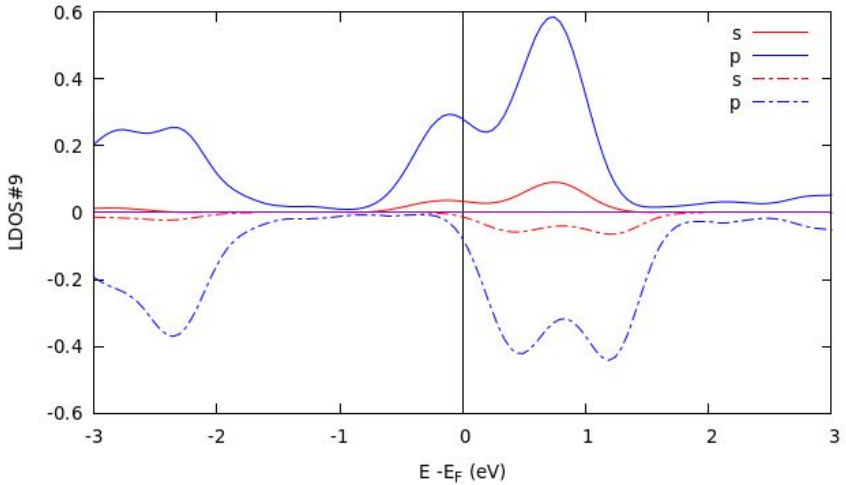


LDOS atom #9 vs LDOS atom #12

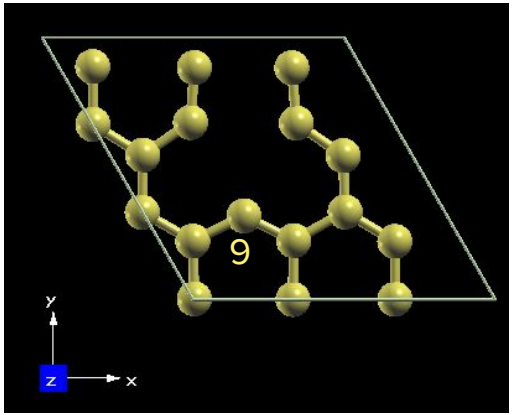


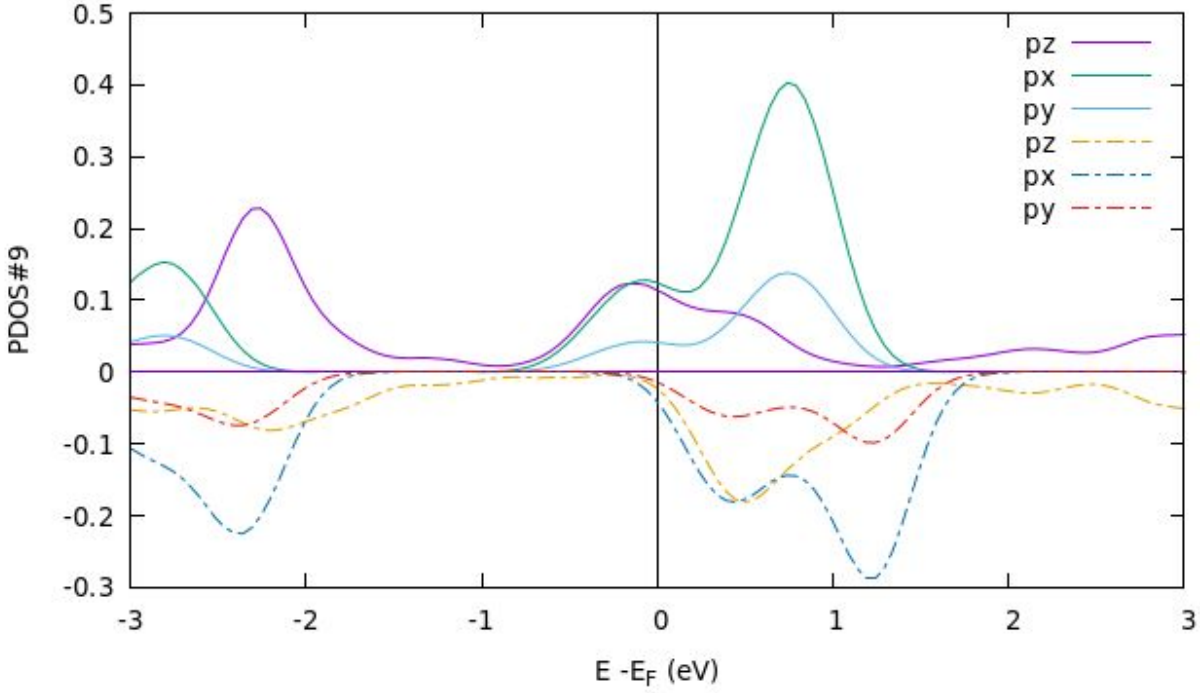
Spin-polarized LDOS atom #12 is quite symmetric, while LDOS of atom #9, near the vacancy, is asymmetric for spin up and spin down distributions. Thus only atoms with unpaired electrons show magnetization.
It can be concluded that the vacancy induced specific spin-density distribution.





PDOS #9


9
y
z
x


PDOS#9
E -E$_F$ (eV)
pz
px
py
pz
px
py
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-3
-2
-1
0
1
2
3

Bibliography

- Faccio et al, *“Electronic and Structural Distortions in Graphene Induced by Carbon Vacancies and Boron Doping”,* J. Phys. Chem. C 2010, 114, 44, 18961–18971
- Jing-Jing Chen et al, *“Magnetic moments in graphene with vacancies”* , 2014 Nanoscale (DOI: 10.1039/c3nr06892g)
- Xian-Qi Dai et al*, “First-principle study of magnetism induced by vacancies in graphene”,* 2011 The European Physical Journal (DOI:10.1140/epjb/e2011-10955-x)