Proyecto final:

Cálculo de dispersión fonónica

Presenta:
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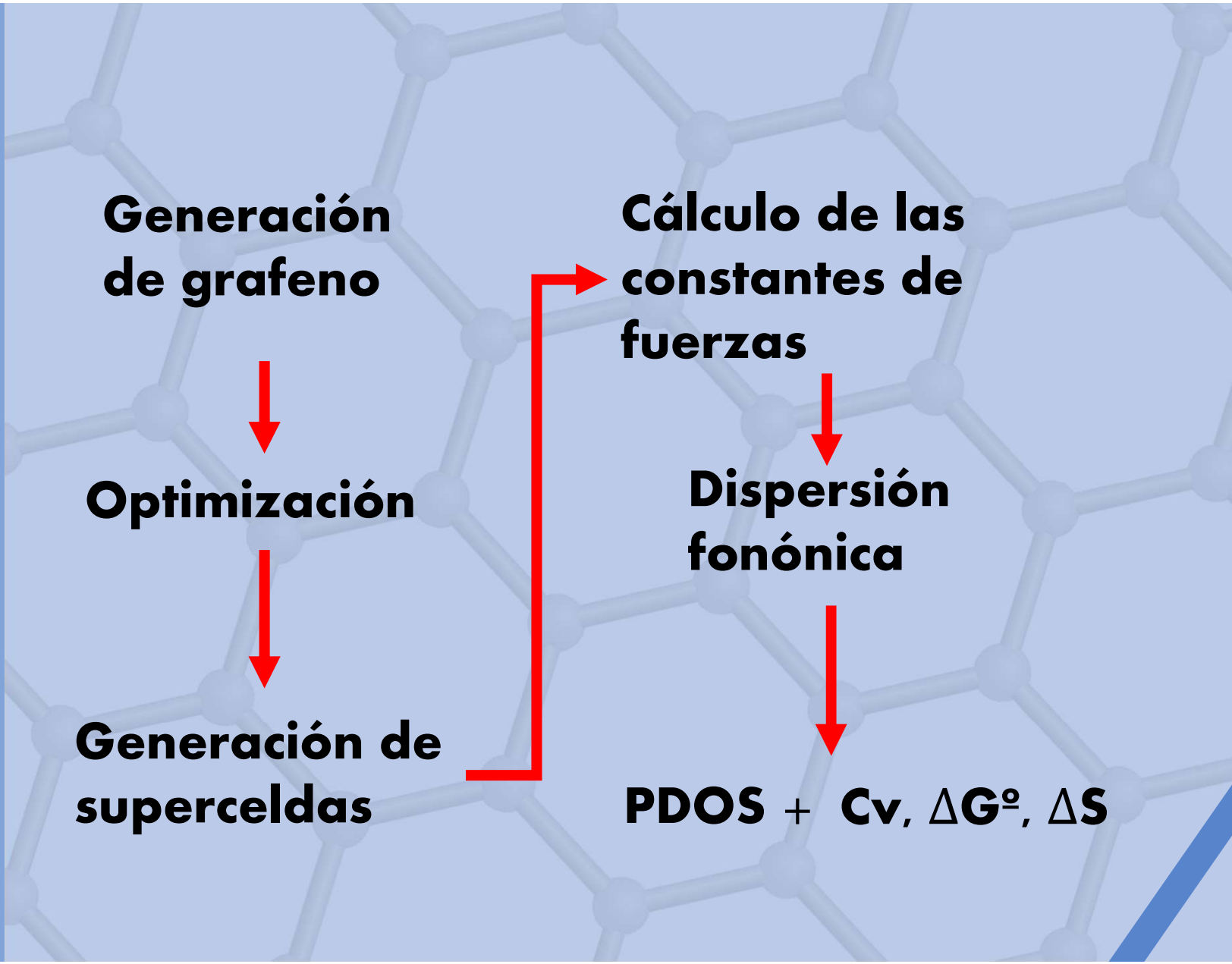
Esquema general:

Objetivo: dispersión fonónica + PDOS + Propiedades térmicas



Generación del grafeno:

sisl

```
import sisl
from sisl import *
import sisl.viz

# Create a graphene structure with the
default parameters.

graphene = sisl.geom.graphene()

# Plot it to see that it is what we
wanted

graphene.plot(axes="x,y")

graphene.write("structure.fdf")
```

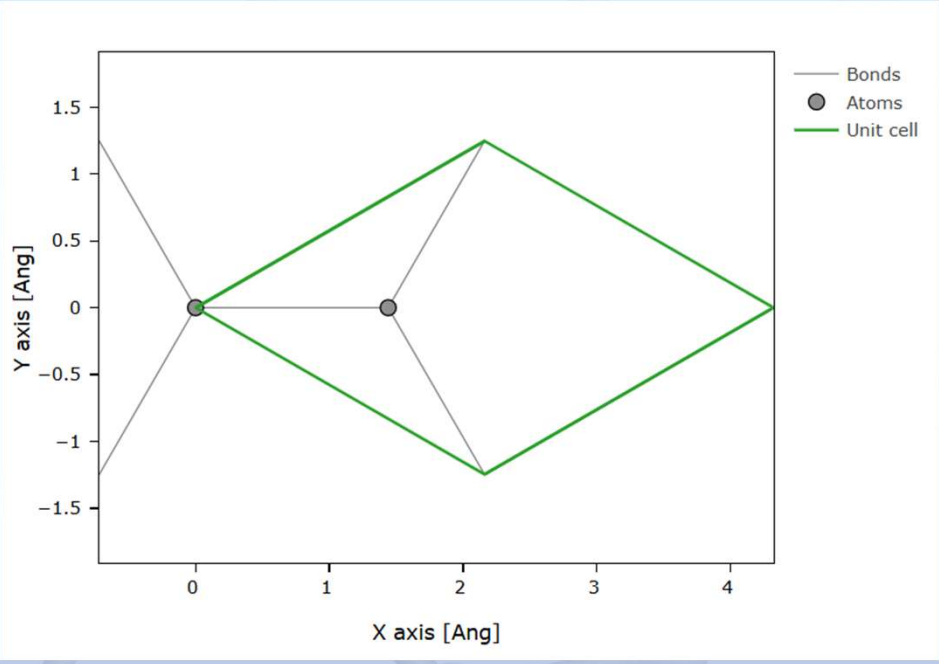


Fig 1. Código y resultados de la generación de grafeno con sisl

Optimización del grafeno

SIESTA

```
# Variable cell relaxation of a crystal (energy minimization)
# https://docs.siesta-project.org/projects/siesta/en/latest/tutorials/basic/structure-optimization/
SystemLabel relaxation

#input structure
%include structure.fdf

#General aspects Calculation (Basis Set and functional)
PAO.BasisSize DZP
PAO.EnergyShift     300 meV
XC.functional     GGA
XC.authors        PBE

%block kgrid_Monkhorst_Pack
   3  0  0  0.0
   0  3  0  0.0
   0  0  3  0.0
%endblock kgrid_Monkhorst_Pack

# General Output
SaveHS true   #Save the Hamiltonian

# Geometry Optimization Options with variable cell
MD.TypeOfRun     CG  #Conjugate Gradient Method
MD.Steps         100  #Number of Steps
MD.MaxForceTol   0.005 eV/Ang
MD.VariableCell       T
MD.MaxStressTol       0.01 GPa  #relax stress
MD.TargetPressure     0.0 GPa

# Geometry Optimization Output

WriteCoorXmol          true         #Save the final coordinates in .xyz format

WriteMDXmol            true         #Writes the coordinates
                                    #of all atoms at all steps
                                    #in a .ANI file
                                    #in xyz format

WriteMDhistory         true         #writes .MDE and .MD files
                                    # with output data from MD simulation
                                    # MDE contains: Temp, energy, volume, pressure
                                    # (human readable)
                                    # MD contains coords vel lattice vectors
                                    # (unformatted; post-process with iomd.f)
```

Fig 2. Archivo de relajación del grafeno

Generación de superceldas:

phonopy

```
phonopy --siesta -d --dim="x x 1"
-c relaxed_graphene.fdf
```

```
NumberOfAtoms 18

%block LatticeVectors
   12.0753500157475209   -6.9717065630235258    0.0000000000000000
   12.0753500157475209    6.9717065630235258    0.0000000000000000
    0.0000000000000000    0.0000000000000000   37.7945227409938056
%endblock LatticeVectors

AtomicCoordinatesFormat  Fractional

LatticeConstant 1.0 Bohr

%block AtomicCoordinatesAndAtomicSpecies
   0.0000000000000000   0.0000000000000000   0.0000000000000000 1
   0.3333333333333333   0.0000000000000000   0.0000000000000000 1
   0.6666666666666666   0.0000000000000000   0.0000000000000000 1
   0.0000000000000000   0.3333333333333333   0.0000000000000000 1
   0.3333333333333333   0.3333333333333333   0.0000000000000000 1
   0.6666666666666666   0.3333333333333333   0.0000000000000000 1
   0.0000000000000000   0.6666666666666666   0.0000000000000000 1
   0.3333333333333333   0.6666666666666666   0.0000000000000000 1
   0.6666666666666666   0.6666666666666666   0.0000000000000000 1
   0.1110328638497653   0.1110328638497653   0.0000000000000000 1
   0.4443661971830986   0.1110328638497653   0.0000000000000000 1
   0.7776995305164319   0.1110328638497653   0.0000000000000000 1
   0.1110328638497653   0.4443661971830986   0.0000000000000000 1
   0.4443661971830986   0.4443661971830986   0.0000000000000000 1
   0.7776995305164319   0.4443661971830986   0.0000000000000000 1
   0.1110328638497653   0.7776995305164319   0.0000000000000000 1
   0.4443661971830986   0.7776995305164319   0.0000000000000000 1
   0.7776995305164319   0.7776995305164319   0.0000000000000000 1
%endblock AtomicCoordinatesAndAtomicSpecies
```

Fig 3. Comando y output de la generación de las superceldas

Generación de desplazamientos:

phonopy

```
NumberOfAtoms 18

%block LatticeVectors
   12.0753500157475209   -6.9717065630235258    0.0000000000000000
   12.0753500157475209    6.9717065630235258    0.0000000000000000
    0.0000000000000000    0.0000000000000000   37.7945227409938056
%endblock LatticeVectors

AtomicCoordinatesFormat  Fractional

NumberOfSpecies 1
%block ChemicalSpeciesLabel
 1 6 C
%endblock ChemicalSpeciesLabel

LatticeConstant 1.0 Bohr

%block AtomicCoordinatesAndAtomicSpecies
   0.0004964682870935   0.0000000000000000   0.0004964682870935 1
   0.3333333333333333   0.0000000000000000   0.0000000000000000 1
   0.6666666666666666   0.0000000000000000   0.0000000000000000 1
   0.0000000000000000   0.3333333333333333   0.0000000000000000 1
   0.3333333333333333   0.3333333333333333   0.0000000000000000 1
   0.6666666666666666   0.3333333333333334   0.0000000000000000 1
   0.0000000000000000   0.6666666666666666   0.0000000000000000 1
   0.3333333333333333   0.6666666666666666   0.0000000000000000 1
   0.6666666666666666   0.6666666666666666   0.0000000000000000 1
   0.1110328638497653   0.1110328638497653   0.0000000000000000 1
   0.4443661971830987   0.1110328638497653   0.0000000000000000 1
   0.7776995305164319   0.1110328638497653   0.0000000000000000 1
   0.1110328638497653   0.4443661971830987   0.0000000000000000 1
   0.4443661971830986   0.4443661971830986   0.0000000000000000 1
   0.7776995305164319   0.4443661971830986   0.0000000000000000 1
   0.1110328638497653   0.7776995305164319   0.0000000000000000 1
   0.4443661971830987   0.7776995305164319   0.0000000000000000 1
   0.7776995305164320   0.7776995305164320   0.0000000000000000 1
%endblock AtomicCoordinatesAndAtomicSpecies
```

Fig 4. Primera celda con desplazamiento

Cálculos de constantes de fuerzas:

SIESTA

\+

Phonopy:

```
siesta < supercell-00x.fdf >
supercell-00x.out
```

```
phonopy -f "disp-001/siesta.FA"
"disp-002/siesta.FA"
```

```
18
2

1
  0.0059950283383723  -0.0034612312154626   0.0187637819667364
   0.0959521465    0.0410973459   -0.1075066472
   0.1901196998   -0.0947156924   -0.0066085746
   0.2598394588    0.0265480396   -0.0063748991
   0.2494908908    0.0450880033   -0.0064860652
   0.3238013628   -0.0903618654    0.0045826107
   0.1691146708   -0.0937609599   -0.0065524569
   0.1798406768   -0.0760529981   -0.0063646279
   0.2390577668    0.0278896837   -0.0066633337
   0.3238015108   -0.0903583662    0.0045818431
  -0.2163121782   -0.0131637192    0.0535456783
  -0.1767921682    0.0059457581   -0.0099422464
  -0.1801097512    0.0489453760    0.0522599894
  -0.2478433102    0.1286494969   -0.0098268098
  -0.3196666592    0.0049403659   -0.0093666412
  -0.1738856492    0.0041878334    0.0025870633
  -0.1438280862   -0.0133227813    0.0521915698
  -0.2484742192    0.1339249139    0.0024984094
  -0.3241061622    0.0045195652    0.0034451382

1
 -0.0059950283383723   0.0034612312154626  -0.0187637819667364
   0.2371064950   -0.0412714137    0.1074827335
   0.1442982390    0.0945165947    0.0063695965
   0.0738025076   -0.0268133270    0.0066081589
   0.0846425466   -0.0449698510    0.0064926005
   0.0098063780    0.0911195924   -0.0045817876
   0.1653875440    0.0941643913    0.0065392825
   0.1552102110    0.0764822100    0.0066121008
   0.0948141770   -0.0272950968    0.0064228857
   0.0098068223    0.0911213461   -0.0045815404
  -0.1178252910    0.0131648293   -0.0536664557
  -0.1574881580   -0.0058581430    0.0099474506
  -0.1535214880   -0.0500070907   -0.0521179183
  -0.0861200259   -0.1299916003    0.0100685269
  -0.0145536356   -0.0053519233    0.0091220741
  -0.1604722470   -0.0042167592   -0.0025857584
  -0.1900872410    0.0140475586   -0.0521873281
  -0.0849200626   -0.1346910943   -0.0026738003
  -0.0098867711   -0.0041502235   -0.0032708212
```

Fig 5. Archivo de fuerzas procesado por phonopy

Cálculo y plot de la dispersión fonónica:

phonopy

```
phonopy -c relaxed_graphene.fdf -p band.conf
```

```
ATOM_NAME = C
DIM = 3 3 1
BAND_POINTS = 101
BAND = 0.0000000000  0.0000000000  0.0000000000
0.6666666667  0.3333333333  0.0000000000
0.5000000000  0.5000000000  0.0000000000
1.0000000000  1.0000000000 0.0000000000
BAND_LABELS = G K M $\Gamma$
```

Fig 6. Archivo band.conf para el cálculo de la dispersión

Cálculo y plot de la PDOS:

phonopy

```
phonopy -p pdos.conf
phonopy -p band-pdos.conf
```

```
ATOM_NAME = C
DIM = 4 4 1
BAND_POINTS = 101
BAND = 0.0000000000  0.0000000000  0.0000000000
0.6666666667  0.3333333333  0.0000000000
0.5000000000  0.5000000000  0.0000000000
1.0000000000  1.0000000000 0.0000000000
DIM = 4 4 1
MP = 20 20 3
PDOS = AUTO
BAND_LABELS = G K M $\Gamma$
```

```
DIM = 3 3 1
MP = 20 20 3
PDOS = AUTO
```

Fig 7. Archivo pdos.conf y band-pdos.conf

Cálculo y plot de la Cv, ΔGº, ΔS

phonopy

```
phonopy -t -p mesh.conf
```

```
DIM = 3 3 1
MP = 20 20 3
```

Fig 8. Archivo mesh.conf

Resultados de la dispersión:

phonopy

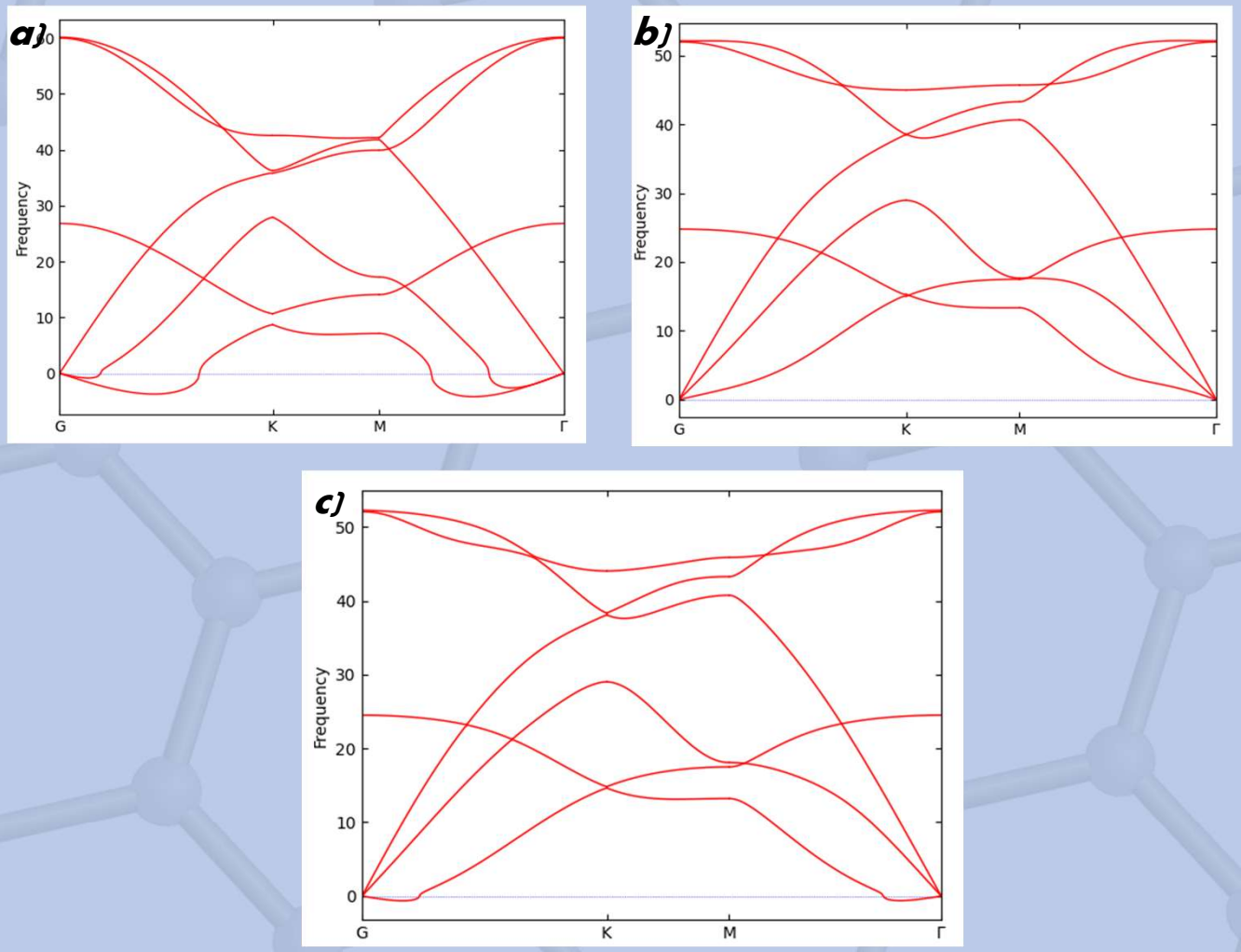


Fig 9. Resultados de la dispersión para las superceldas de a) 2x2x1, b) 4x4x1 y c) 5x5x1

Otros resultados... :

phonopy

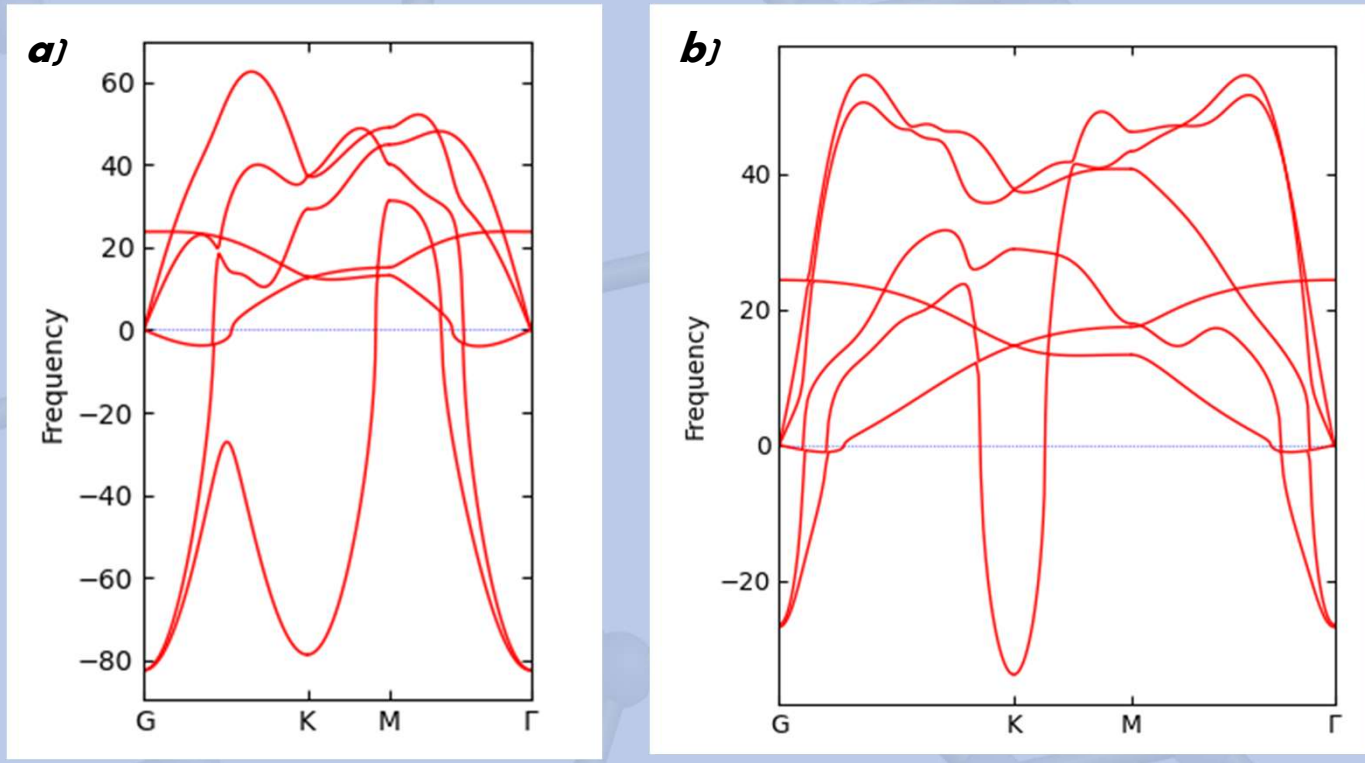


Fig 10. Resultados de la dispersión para las superceldas de a) 3x3x1 y b) 6x6x1

Resultados de la PDOS:

phonopy

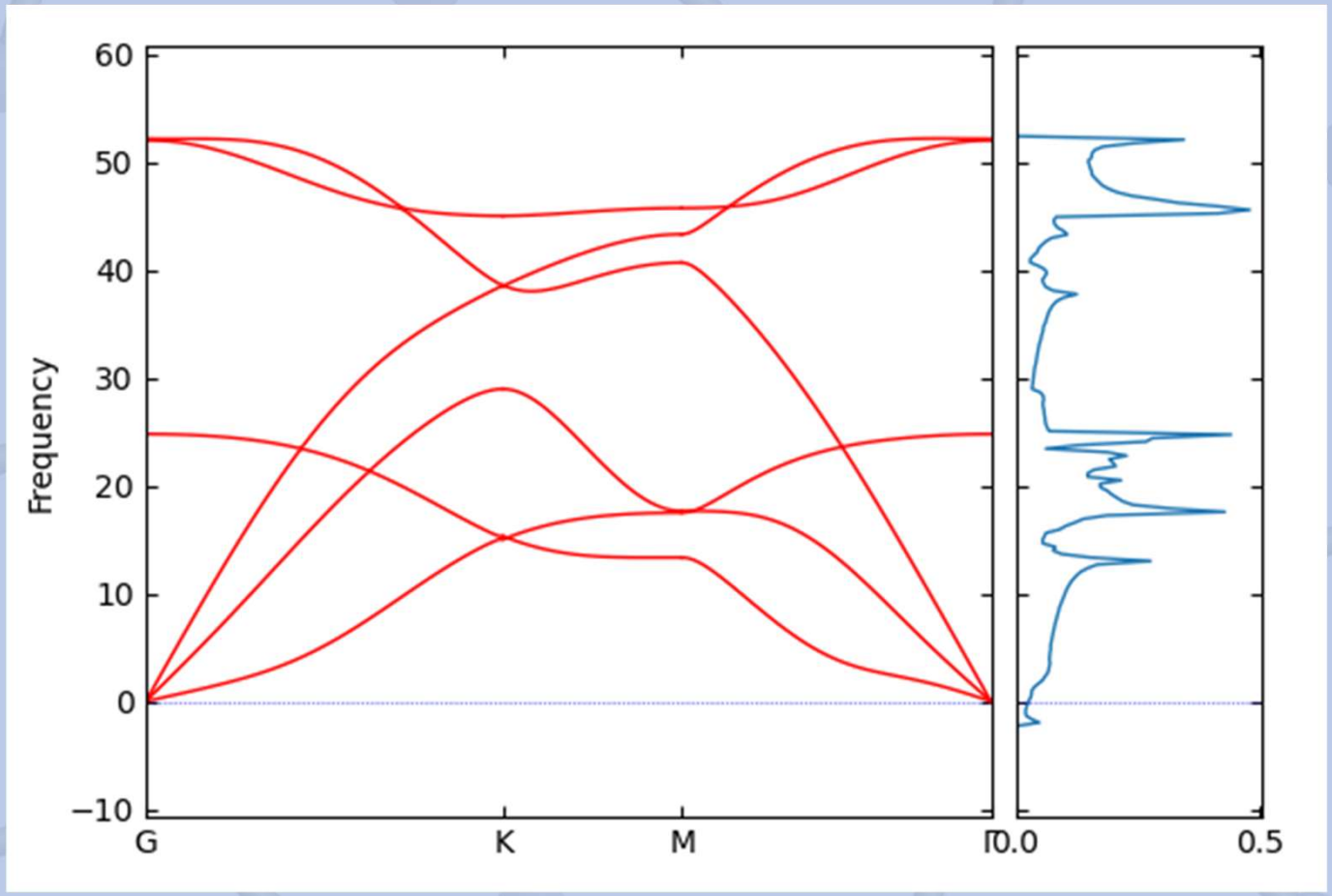


Fig 11. Resultados de la PDOS y dispersión para la supercelda de 4x4x1

Resultados de la Cv, ΔGº, ΔS:

phonopy

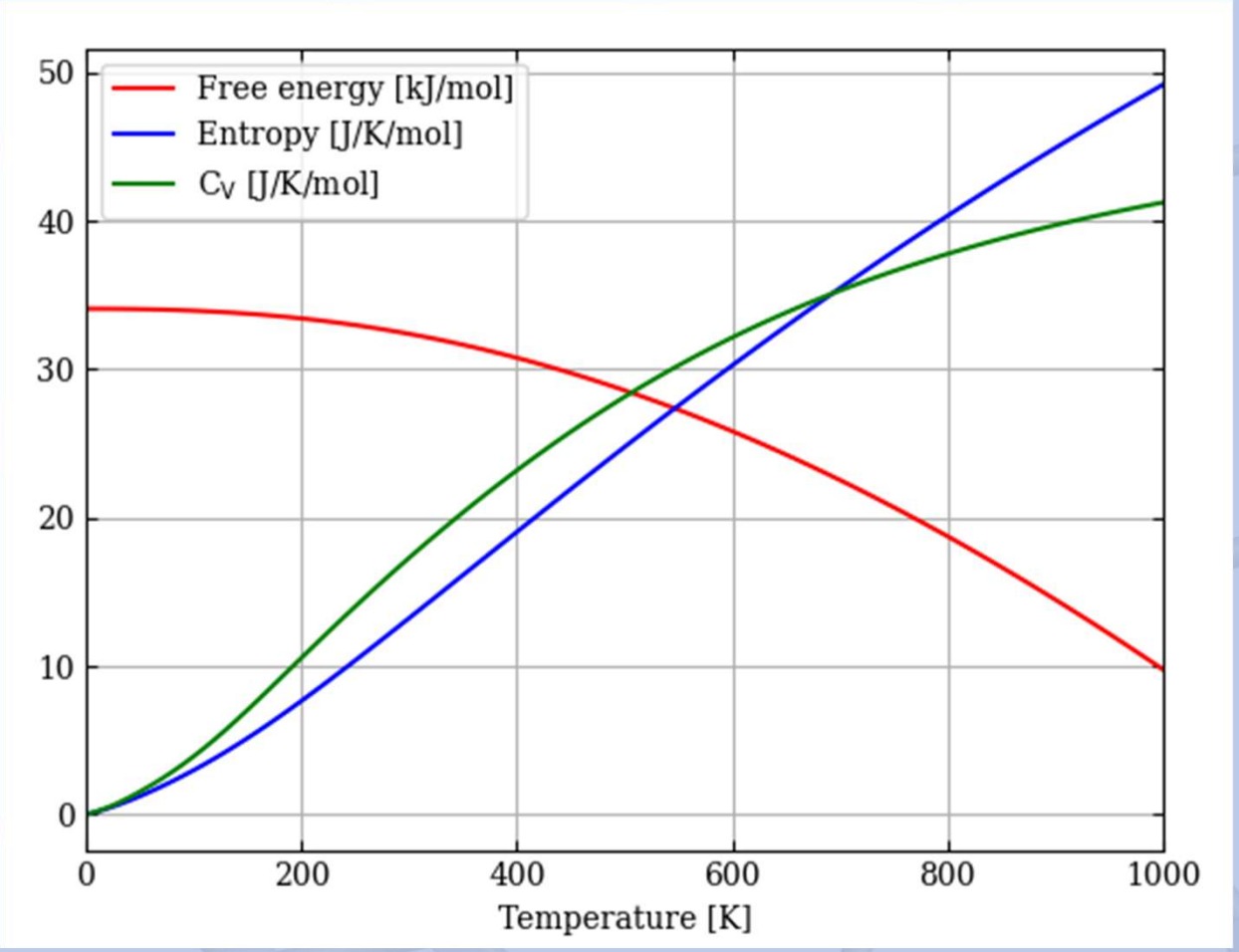
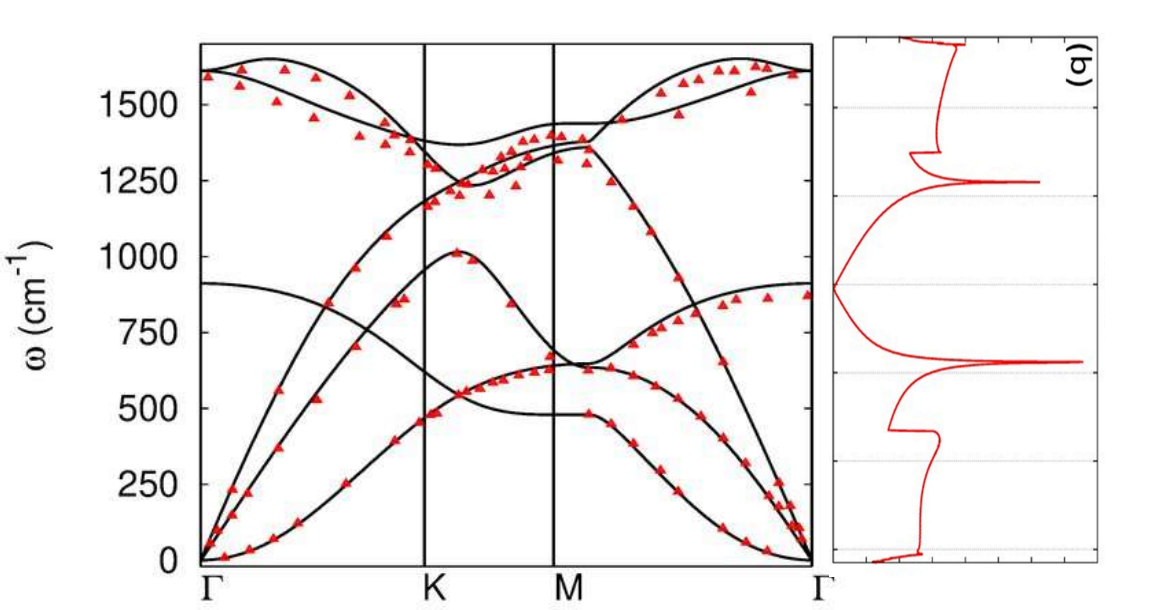


Fig 12. Resultados de la* Cv, ΔGº, ΔS *para la supercelda de 4x4x1

Conclusiones

Conclusiones



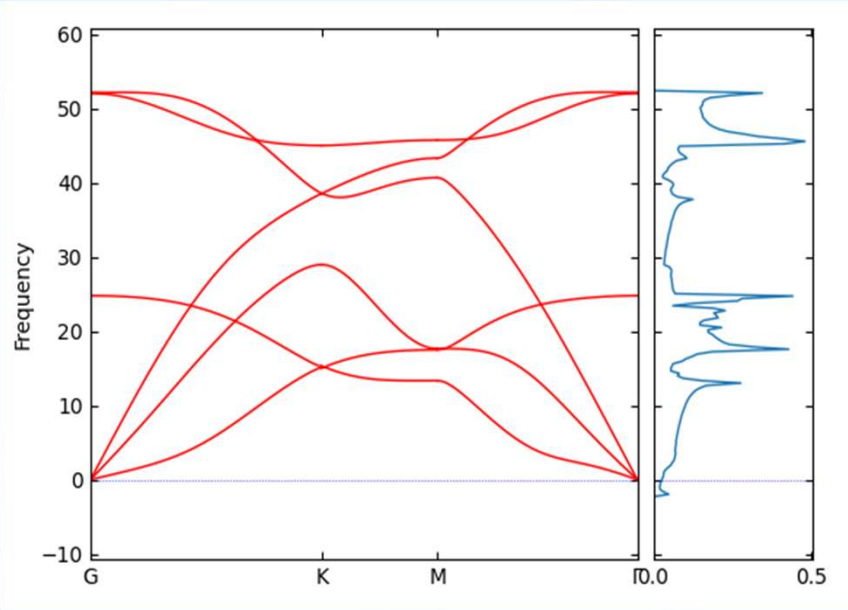
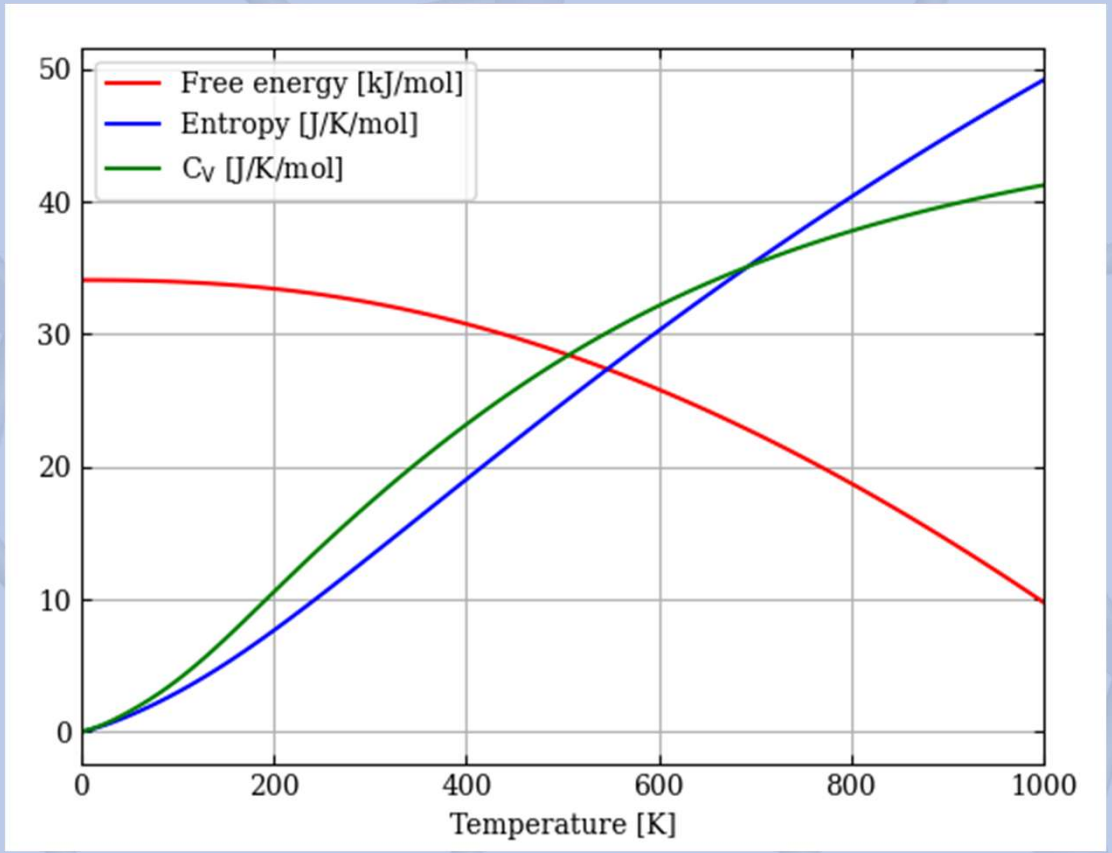


Fig 13. Comparación de resultados experimentales con SIESTA + phonopy

"Significant reduction of lattice thermal conductivity in suspended graphene by charge doping" Ajit Jena, Wu Li

Conclusiones



Gracias!