

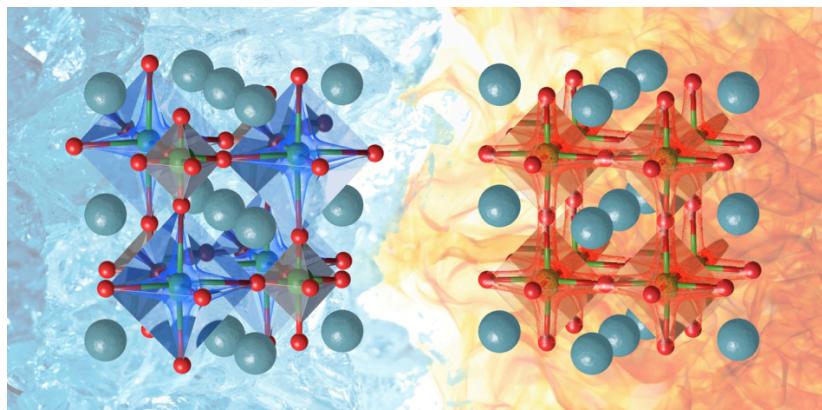
Sesión Práctica de Computación con Métodos Ab Initio en Ciencia de Materiales

Alejandro Molina Sánchez
Alberto García Cristóbal

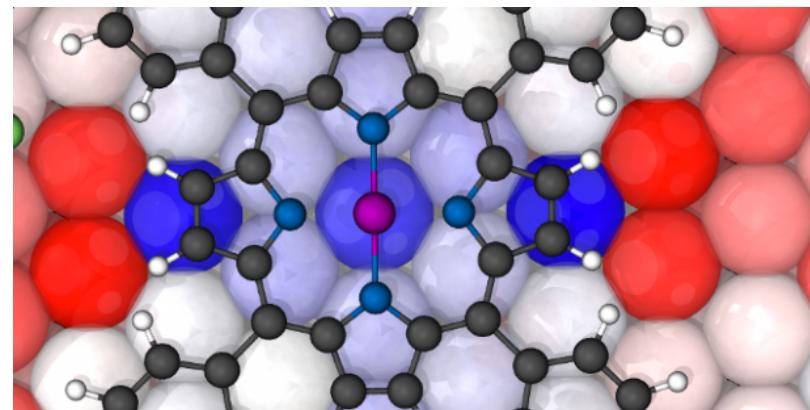
Curso de verano 2019
Instituto de Ciencia de Materiales de la
Universidad de Valencia

Códigos ab initio

*“**ABINIT** software suite to calculate the optical, mechanical, vibrational, and other observable properties of materials. Starting from the quantum equations of density functional theory”*

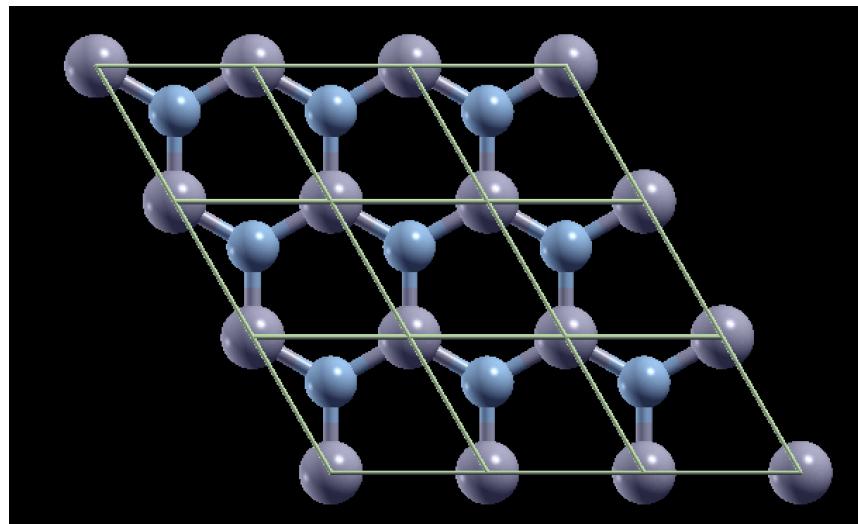
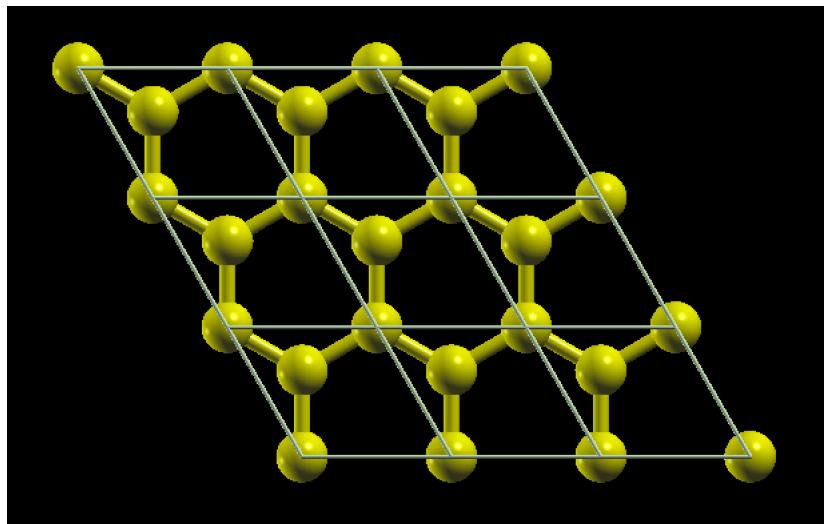


phase-transition in nickelates (ABINIT website)



magnetic molecules (Quantum Espresso website)

Grafeno y Nitruro de Boro



The Kohn-Sham problem

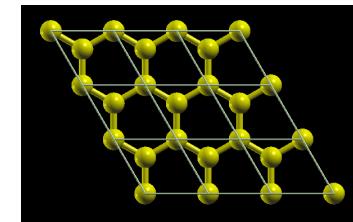
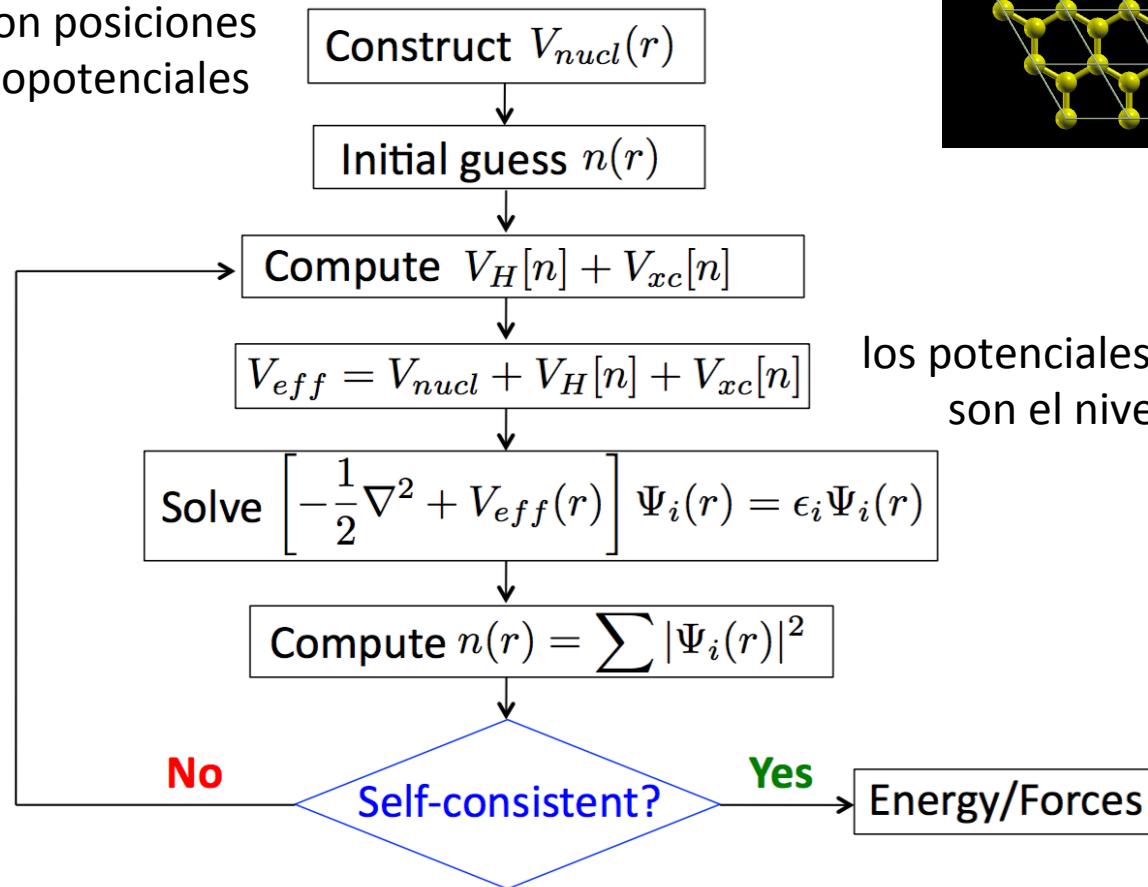
$$\left[-\frac{1}{2} \nabla^2 + V_{nucl}(r) + V_H[n] + V_{xc}[n] \right] \Psi_i(r) = \epsilon_i \Psi_i(r)$$

$$\Psi_i(r) \longrightarrow n(r) \longrightarrow H[n]$$



Iterative solution

los únicos input son posiciones atómicas y pseudopotenciales



los potenciales de interacción
son el nivel de teoría

bn.scf input file

```
bn - vim - 159x43
1 &control
2     calculation = 'scf'
3         prefix = 'pw'
4         verbosity = 'high'
5         wf_collect = .true.
6         pseudo_dir = '.'
7 /&end
8 &system
9     celldm(1) = 4.7
10    celldm(3) = 2.55319148936
11        ecutwfc = 40
12        ibrav = 4
13        nat = 2
14        ntyp = 2
15 /&end
16 &electrons
17     conv_thr = 1e-08
18 /&end
19 &ions
20     ion_dynamics = 'bfgs'
21 /&end
22 &cell
23     cell_dofree = '2Dxy'
24     cell_dynamics = 'bfgs'
25 /&end
26 ATOMIC_SPECIES
27   B  10.811  B_r.upf
28   N  10.811  N_r.upf
29 ATOMIC_POSITIONS { crystal }
30   B  0.000000000  0.000000000  0.500000000
31   N  0.333333333  0.666666667  0.500000000
32 K_POINTS { automatic }
33   3  3  1  0  0  0
```

control variables. Tipo de cálculo (auto-consistente, bandas, relajación, etc.).

system variables. Relacionadas con la estructura cristalina, simetría, número de átomos, tamaño de la base, etc.

ions and cell variables. Solo se utilizan para optimizar las posiciones atómicas y los parámetros de red

Definición de especies atómicas y posiciones de los átomos

Definción del mallado en k. Uniforme o lista de puntos

scf calculation

```
bravais-lattice index      =          4
lattice parameter (alat)   =      4.7000  a.u.
unit-cell volume           =    229.5660 (a.u.)^3
number of atoms/cell       =          2
number of atomic types     =          2
number of electrons         =      8.00
number of Kohn-Sham states=          4
kinetic-energy cutoff       =      40.0000  Ry
charge density cutoff       =    160.0000  Ry
convergence threshold       =    1.0E-08
mixing beta                 =      0.7000
number of iterations used  =          8 plain      mixing
Exchange-correlation        = PBE ( 1 4 3 4 0)

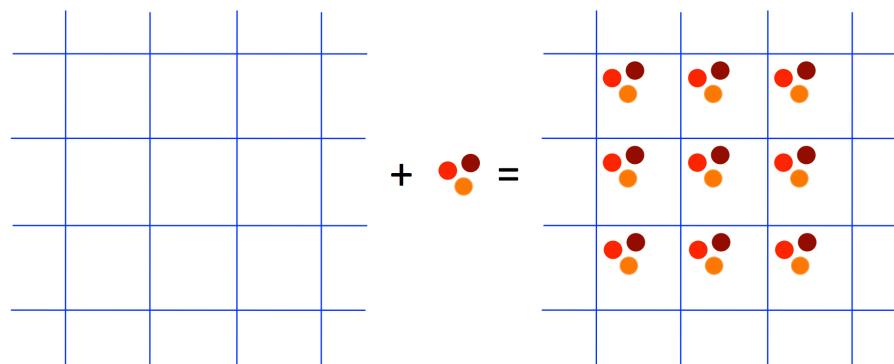
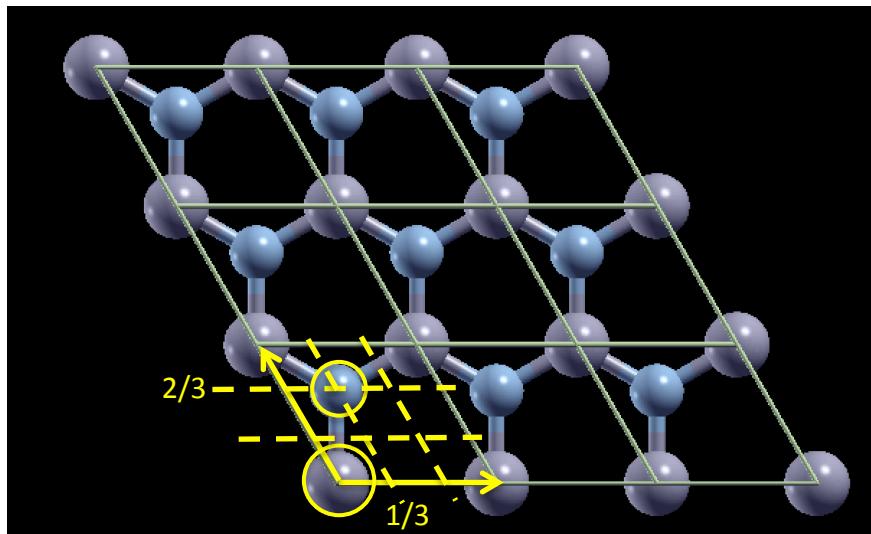
celldm(1)= 4.700000 celldm(2)= 0.000000 celldm(3)= 2.553191
celldm(4)= 0.000000 celldm(5)= 0.000000 celldm(6)= 0.000000

crystal axes: (cart. coord. in units of alat)
  a(1) = ( 1.000000  0.000000  0.000000 )
  a(2) = (-0.500000  0.866025  0.000000 )
  a(3) = ( 0.000000  0.000000  2.553191 )

reciprocal axes: (cart. coord. in units 2 pi/alat)
  b(1) = ( 1.000000  0.577350 -0.000000 )
  b(2) = ( 0.000000  1.154701  0.000000 )
  b(3) = ( 0.000000 -0.000000  0.391667 )
```

scf calculation. parameters

```
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 2     calculation = 'scf'
 3         prefix = 'pw'
 4         verbosity = 'high'
 5         wf_collect = .true.
 6         pseudo_dir = '.'
 7 /&end
 8 &system
 9         celldm(1) = 4.7
10         celldm(3) = 2.55319148936
11             ecutwfc = 40
12             ibrav = 4
13             nat = 2
14             ntyp = 2
15 /&end
16 &electrons
17     conv_thr = 1e-08
18 /&end
19 &ions
20     ion_dynamics = 'bfgs'
21 /&end
22 &cell
23     cell_dofree = '2Dxy'
24     cell_dynamics = 'bfgs'
25 /&end
26 ATOMIC_SPECIES type of atom/pseudopotential
27     B 10.811      B_r.upf
28     N 10.811      N_r.upf
29 ATOMIC_POSITIONS { crystal }
30     B  0.0000000000  0.0000000000  0.5000000000
31     N  0.3333333333  0.6666666667  0.5000000000
32 K_POINTS { automatic }    position
33     3 3 1 0 0 0
```

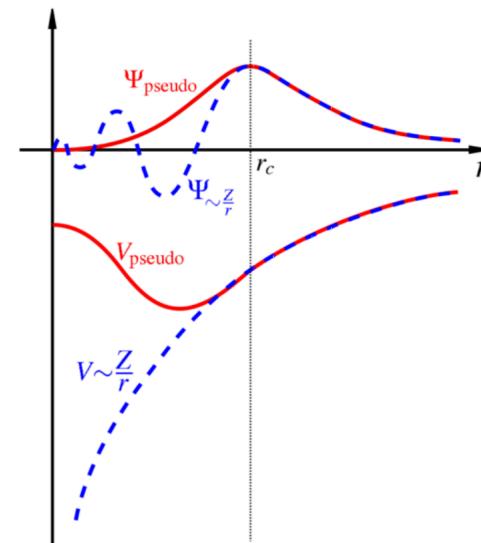


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8 &system
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10    celldm(3) = 2.55319148936
11    ecutwfc = 40
12    ibrav = 4
13    nat = 2  Energy cutoff
14    ntyp = 2
15 /&end
16 &electrons
17     conv_thr = 1e-08
18 /&end
19 &ions
20     ion_dynamics = 'bfgs'
21 /&end
22 &cell
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32 K_POINTS { automatic }
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```

$$\Psi_{\mathbf{k},n}(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{G}} c_{\mathbf{k},n}^{\mathbf{G}} e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}}$$

$$\frac{\hbar^2}{2m} |\mathbf{k} + \mathbf{G}|^2 \leq E_{cut}$$



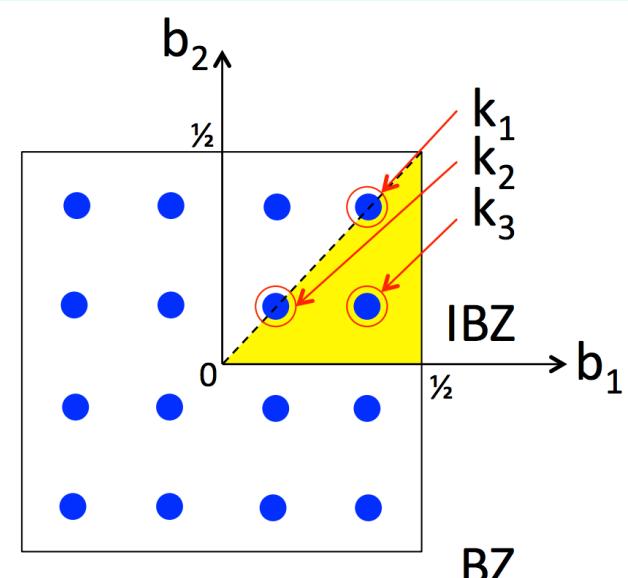
scf calculation. parameters

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32 K_POINTS { automatic }
33   3 3 1 0 0 0
```

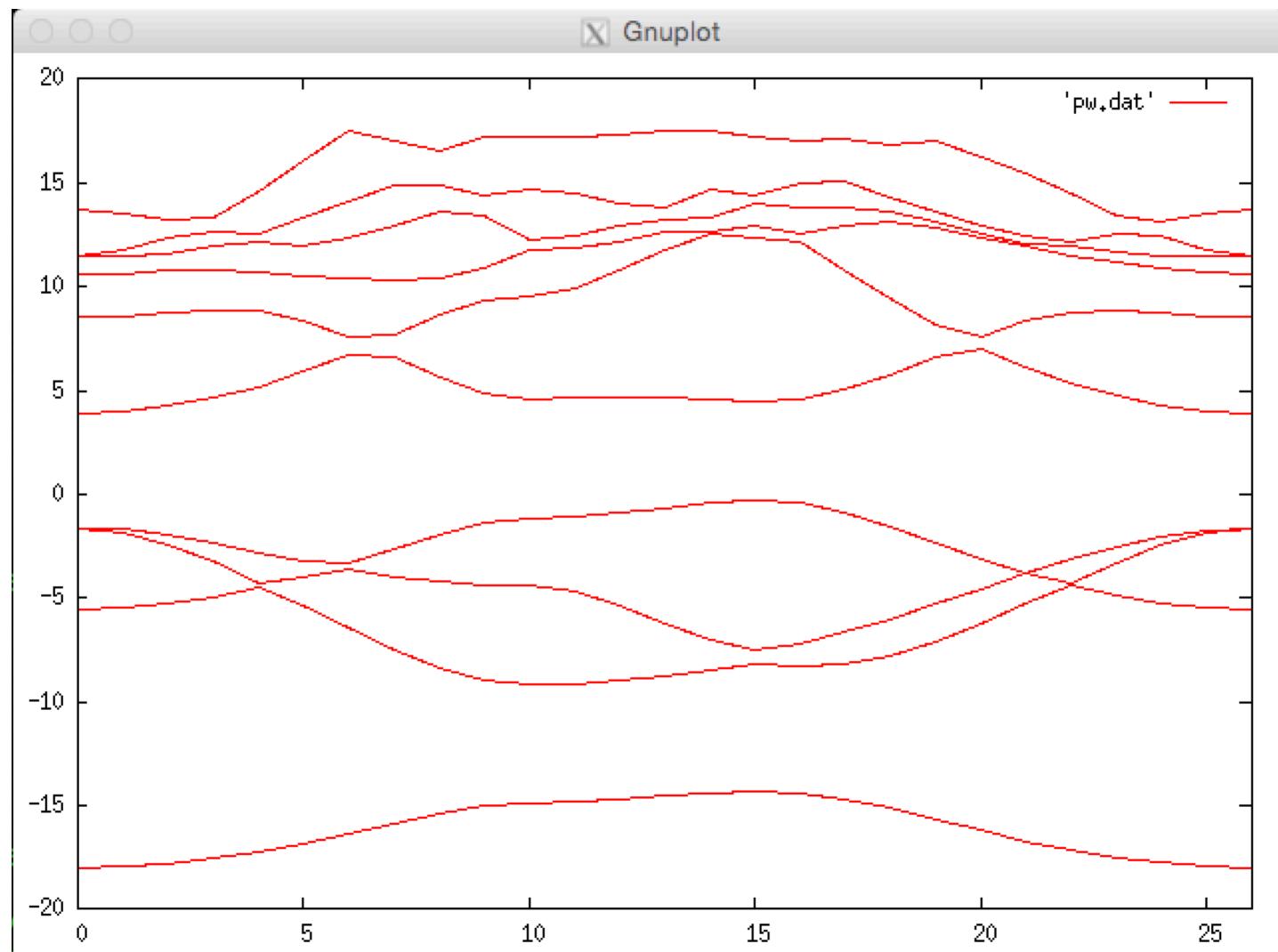
k-point grid

$$n(\mathbf{r}) = \frac{1}{\Omega_{BZ}} \sum_i \int_{BZ} |\Psi_{i,\mathbf{k}}(\mathbf{r})|^2 f(\epsilon_{i,\mathbf{k}} - \epsilon_F) d\mathbf{k}$$

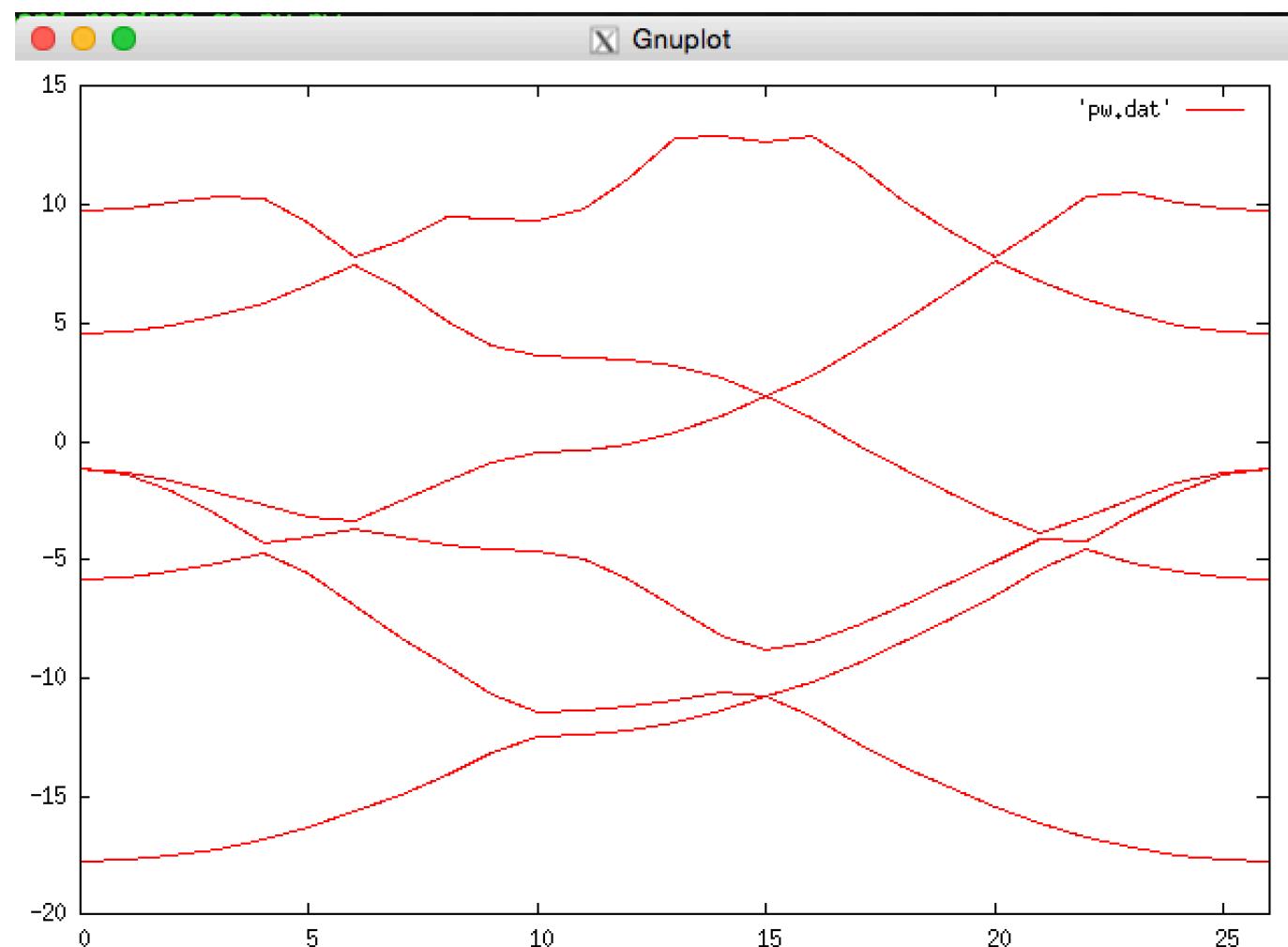
$$\frac{1}{\Omega_{BZ}} \int_{BZ} d\mathbf{k} \rightarrow \sum_{\mathbf{k}} \omega_{\mathbf{k}}$$



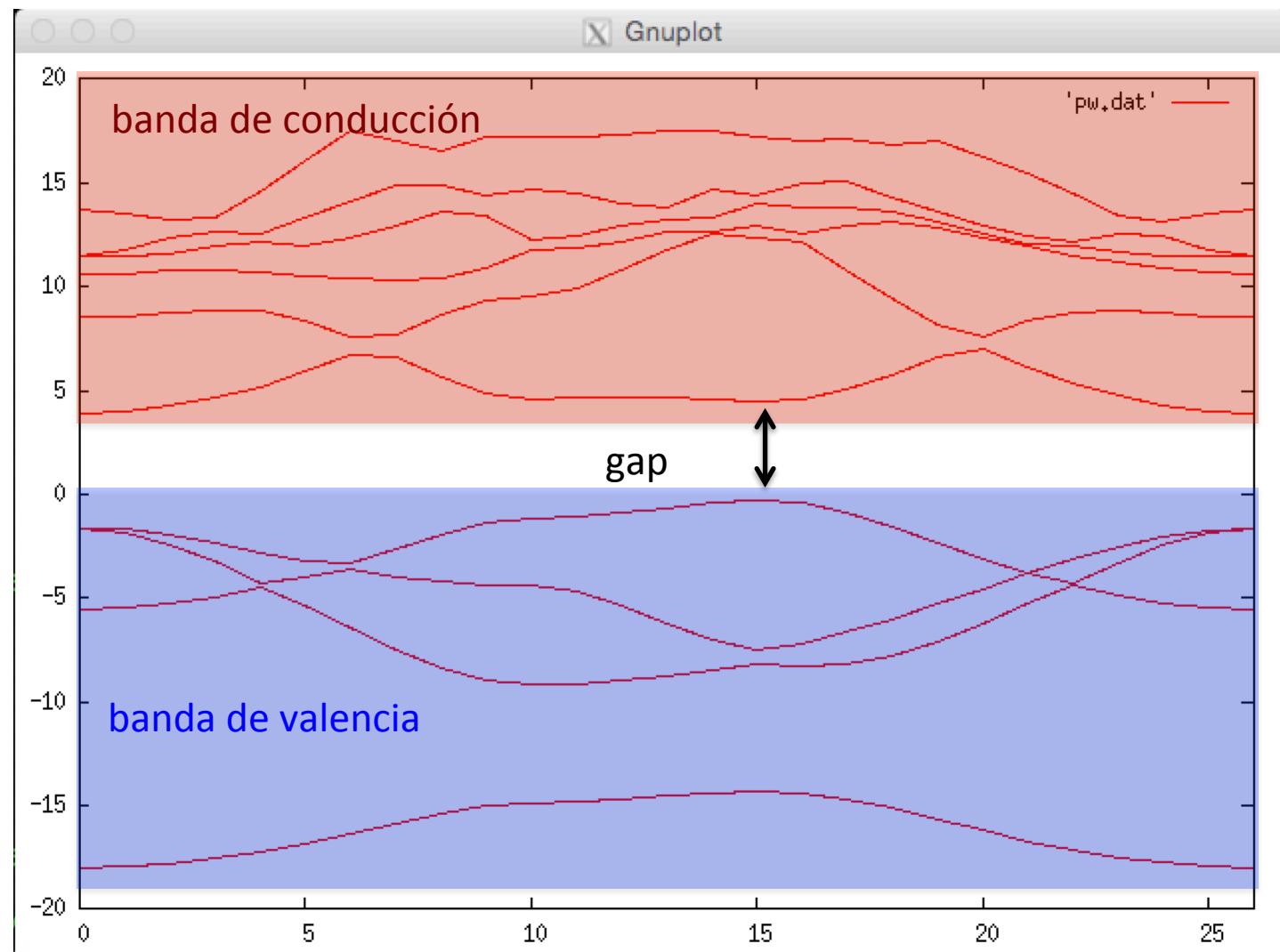
Estructura de bandas. BN



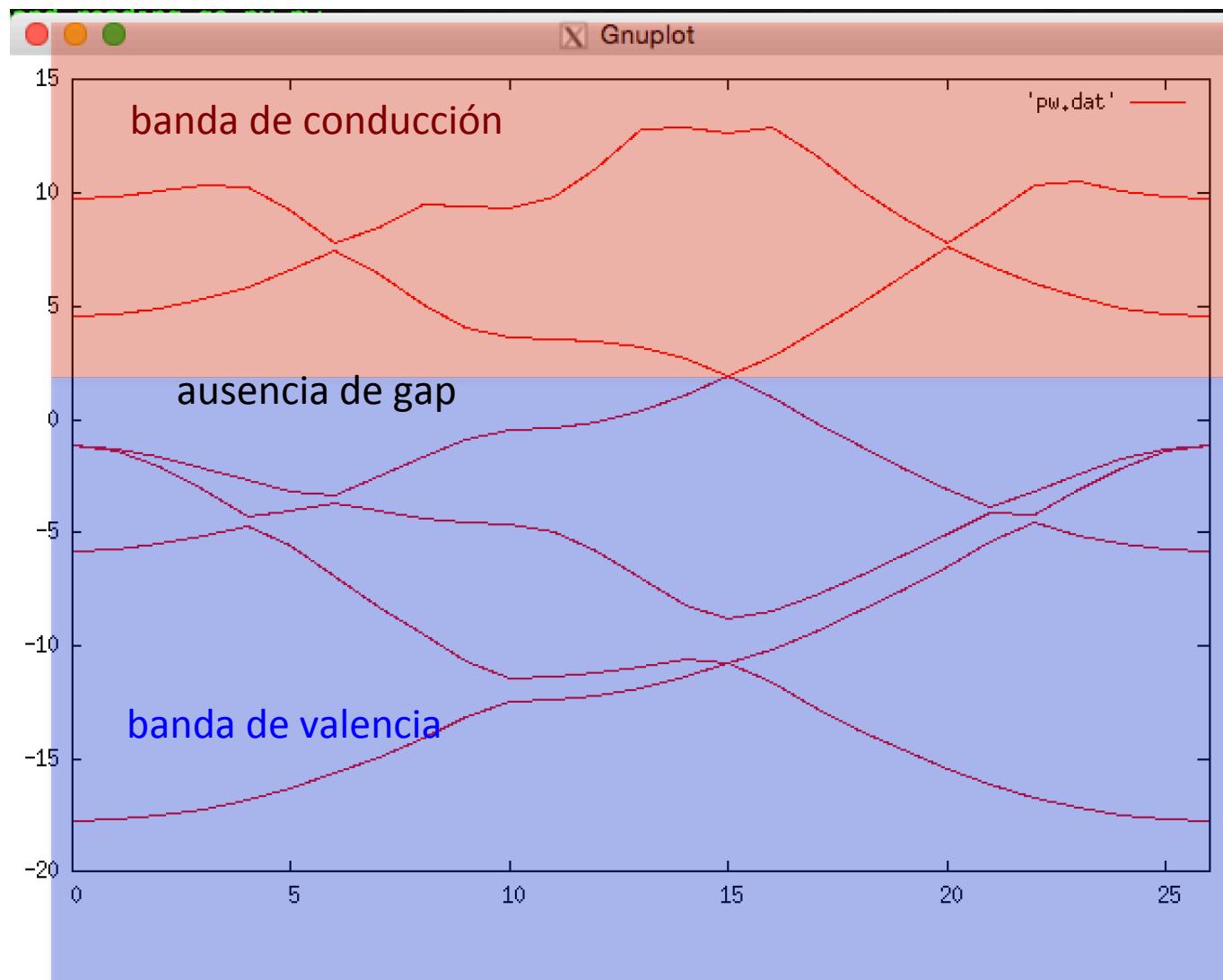
Estructura de bandas. Grafeno



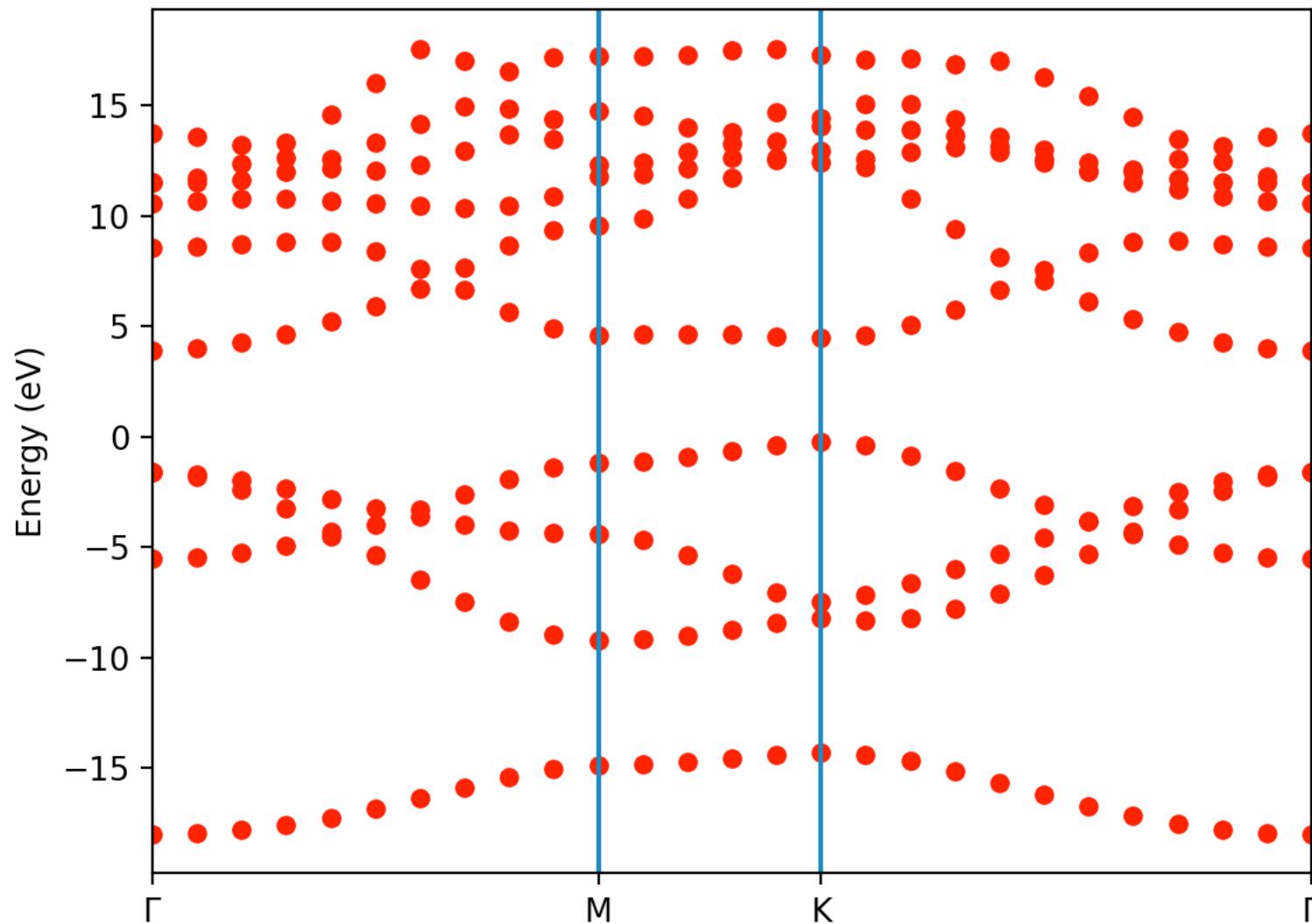
Estructura de bandas. BN



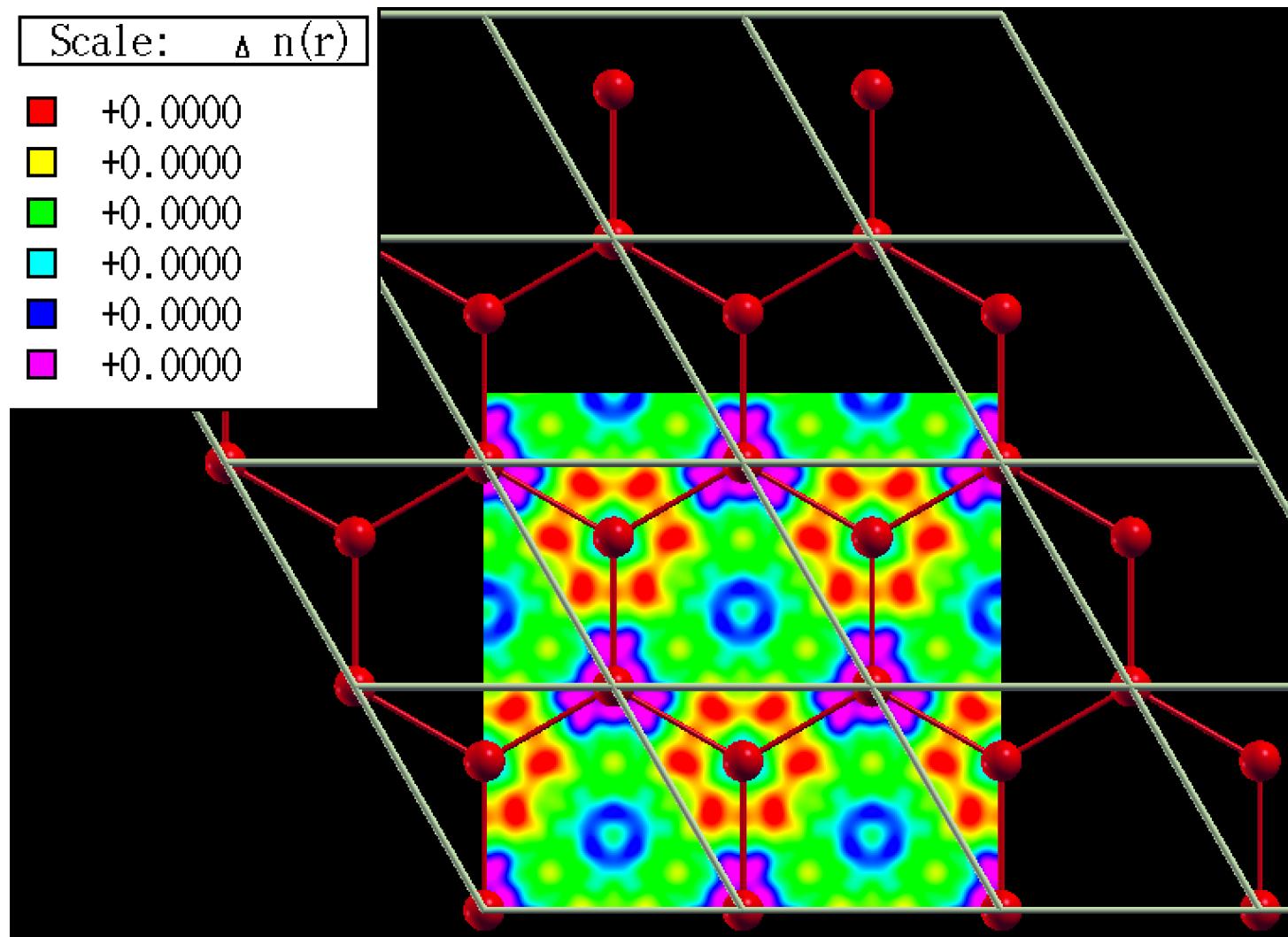
Estructura de bandas. Grafeno



Estructura de bandas. BN



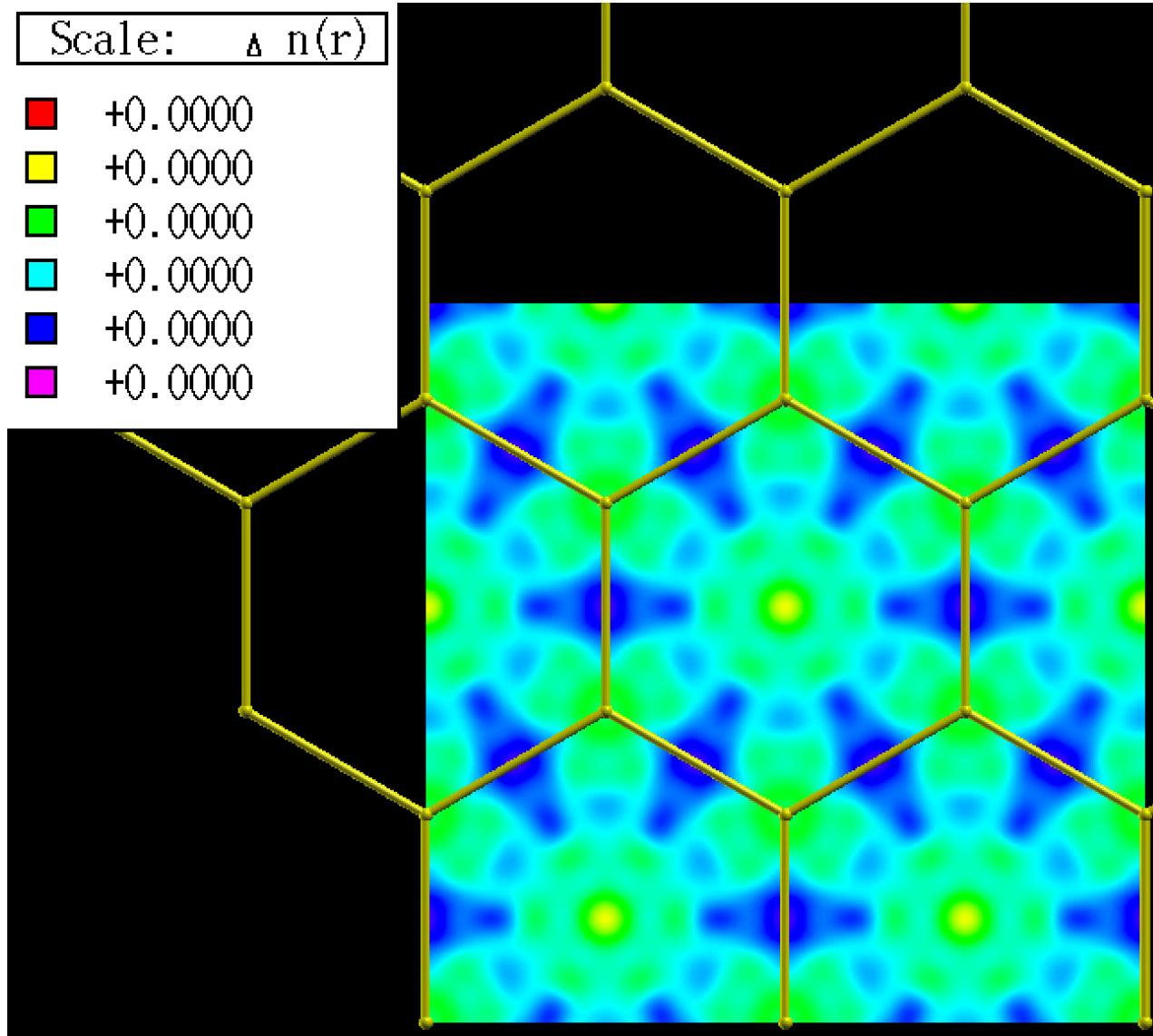
electronic density



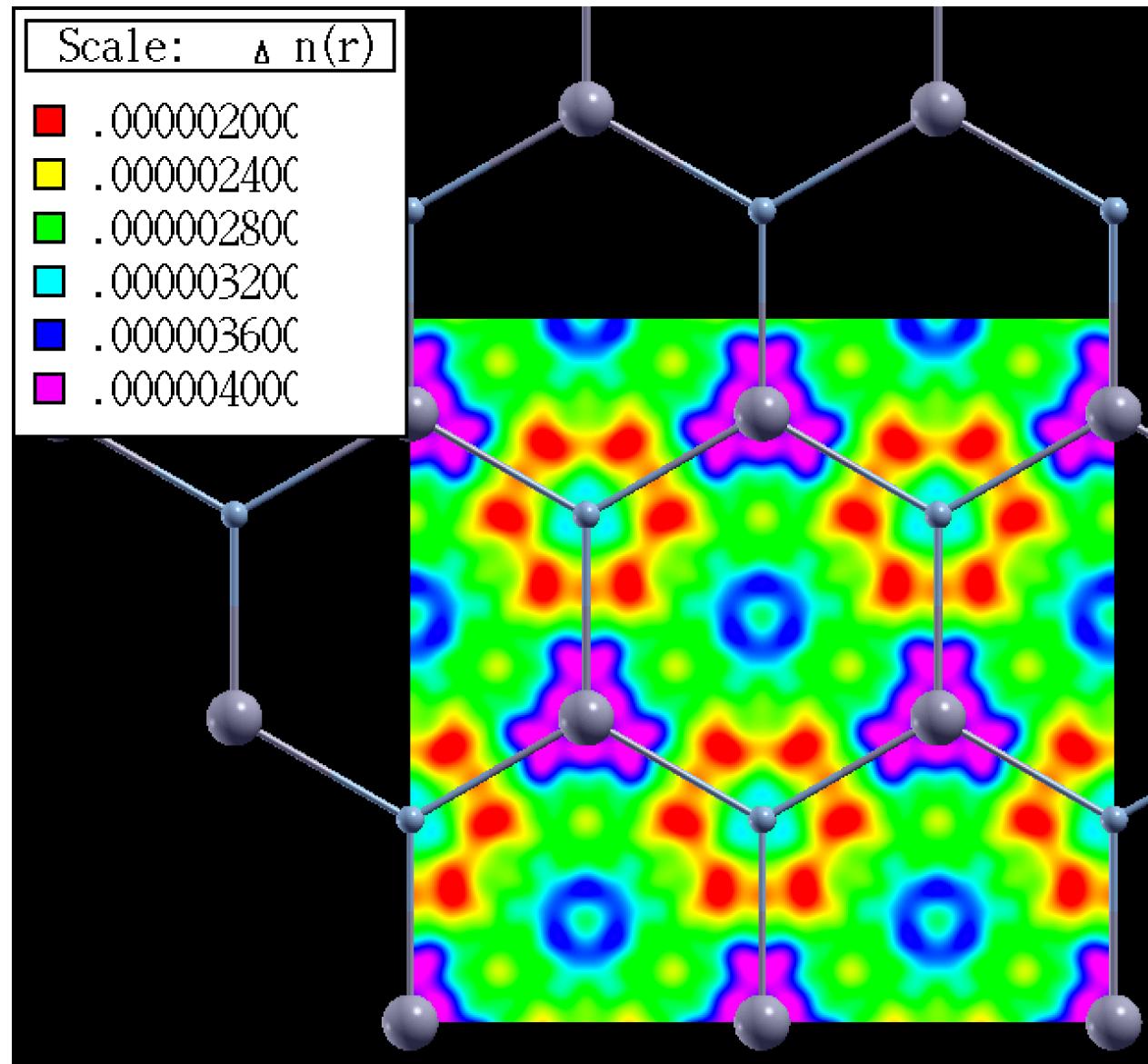
electronic density

Scale: $\Delta n(r)$

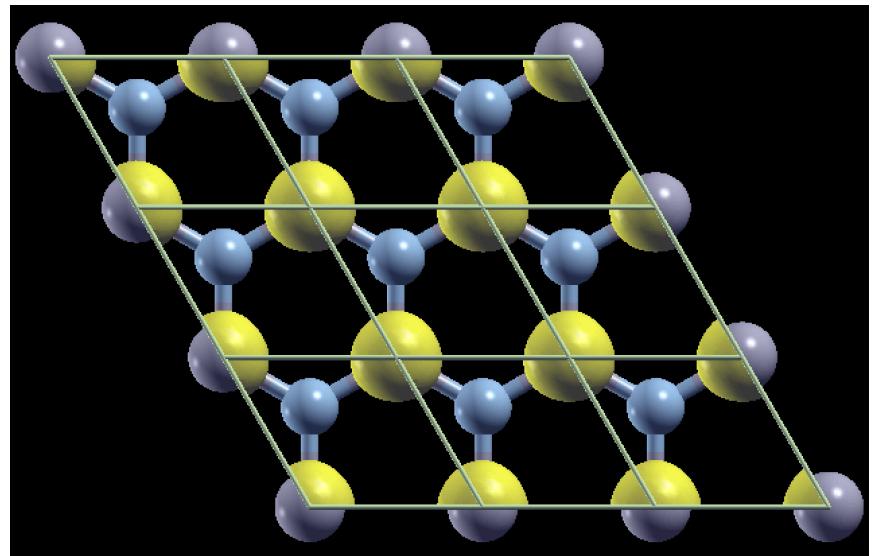
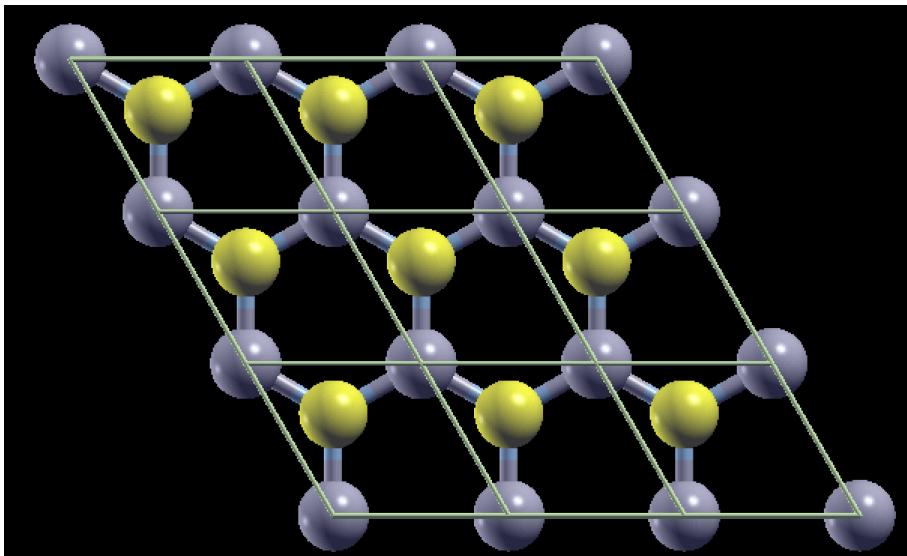
- +0.0000
- +0.0000
- +0.0000
- +0.0000
- +0.0000
- +0.0000



electonic density

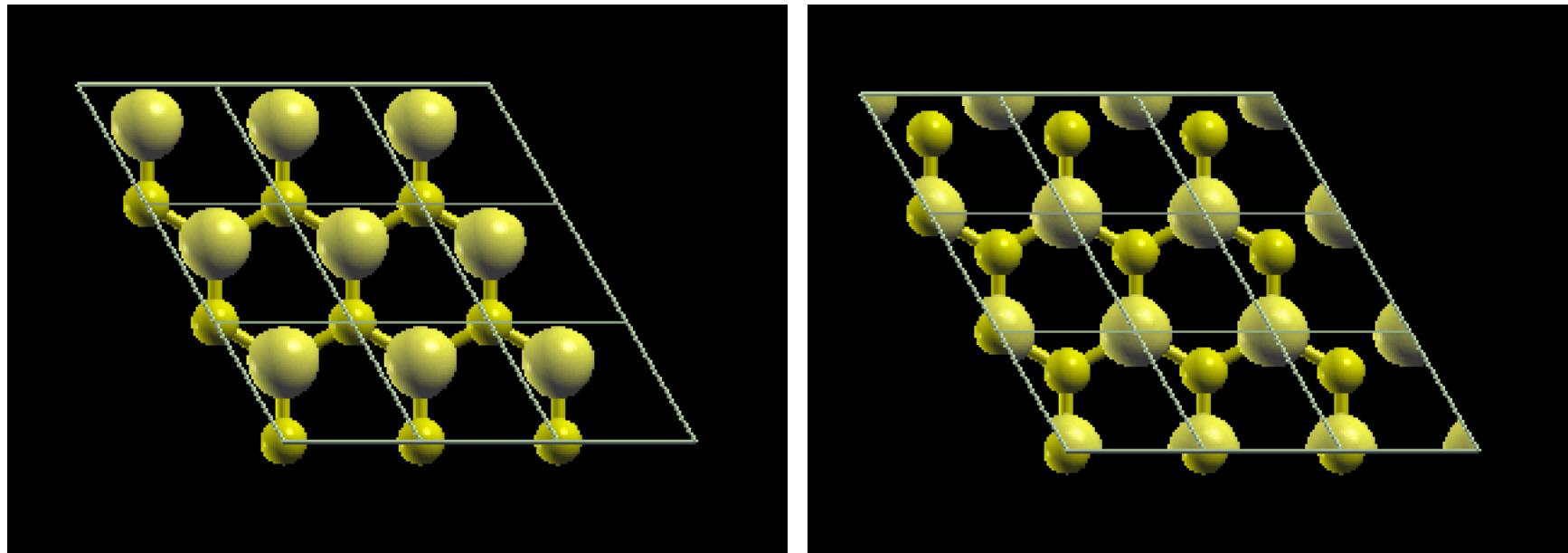


wave functions



valence and conduction band state?

wave functions



valence and conduction band state?

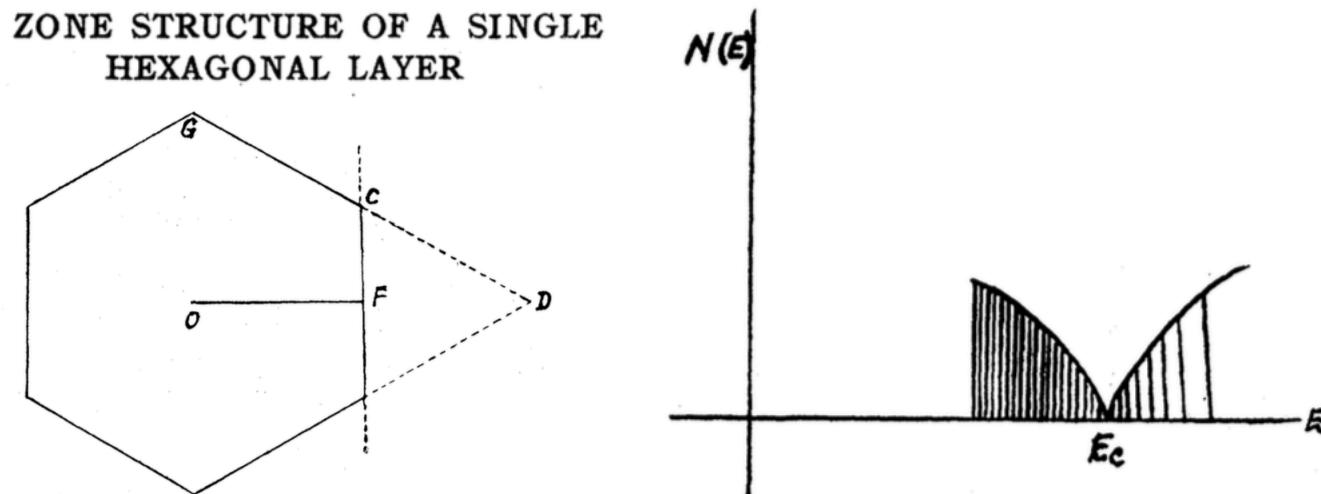
The Band Theory of Graphite

P. R. WALLACE*

National Research Council of Canada, Chalk River Laboratory, Chalk River, Ontario

(Received December 19, 1946)

The structure of the electronic energy bands and Brillouin zones for graphite is developed using the "tight binding" approximation. Graphite is found to be a semi-conductor with zero activation energy, i.e., there are no free electrons at zero temperature, but they are created at higher temperatures by excitation to a band contiguous to the highest one which is normally filled. The electrical conductivity is treated with assumptions about the mean free path. It is found to be about 100 times as great parallel to as across crystal planes. A large and anisotropic diamagnetic susceptibility is predicted for the conduction electrons; this is greatest for fields across the layers. The volume optical absorption is accounted for.



The Nobel Prize in Physics 2010

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Physics for 2010 to

Andre Geim

University of Manchester, UK

and

Konstantin Novoselov

University of Manchester, UK

"for groundbreaking experiments regarding the two-dimensional material graphene"