guido.fratesi@unimi.it

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Structural optimizations

Guido Fratesi (Università di Milano)

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guido.fratesi@unimi.it

Acetylene molecule (C_2H_2)

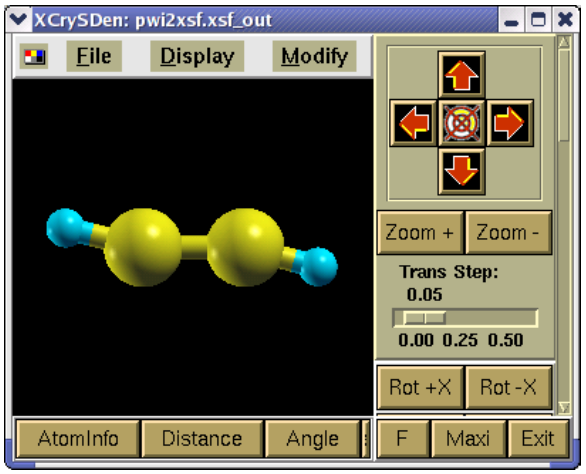
We want to use pw.x to find the optimized geometry of acetylene.

Let us suppose we have the following guess for the structure (coordinates in atomic units):

```
C       0.000000000     0.000000000     0.000000000
C       2.100000000     0.000000000     0.000000000
H      -1.600000000     0.400000000     0.000000000
H       3.600000000    -0.400000000     0.000000000
```

pw.x adopts periodic boundary conditions.
We can put the molecule in a large box, whose size is a convergency parameter.

Here, we choose a cube of side length 12 a.u. for quickness. Then:



1) Prepare the input file for the SCF calculation
   (see next slide for other details), use PWgui if you prefer

2) Visualize the structure with XcrySDen

```
xcrysden --pwi acetylene.scf.in
```

3) Run the SCF calculation and look at forces on atoms.

```
pw.x < acetylene.scf.in > acetylene.scf.out
```

C_2H_2 SCF: the input


```
 &CONTROL
                  calculation = 'scf' ,
                 restart_mode = 'from_scratch' ,
                      outdir = 'your directory for temporary files/' ,
 /
 &SYSTEM
                       ibrav = 1,
                   celldm(1) = 12.D0,
                         nat = 4,
                        ntyp = 2,
                     ecutwfc = 25.0D0 ,
                     ecutrho = 160.0D0 ,
                       nosym = .true. ,
                 occupations = 'smearing' ,
                     degauss = 0.005D0 ,
 /
 &ELECTRONS
                    conv_thr = 1.D-7 ,
                 mixing_beta = 0.5D0 ,
 /
ATOMIC_SPECIES
    H    1.00000  H.US_PBE.RRKJ3.UPF
    C   12.00000  C.US_PBE.RRKJ3.UPF
ATOMIC_POSITIONS bohr
    C      0.000000000    0.000000000    0.000000000    0   0   0
    C      2.100000000    0.000000000    0.000000000    1   1   1
    H     -1.600000000    0.400000000    0.000000000    1   1   1
    H      3.600000000   -0.400000000    0.000000000    1   1   1
K_POINTS gamma
```

Change this!

Why do we treat acetylene as a metal?

Do you have these pseudopotentials?

This atom is locked

Gamma point only is sufficient for the molecule-in-a-box approach

C_2H_2 SCF: the output

From the output file:

```
     Forces acting on atoms (Ry/au):

     atom    1 type  2   force =     0.04225946   -0.07108502    0.00000000
     atom    2 type  2   force =    -0.29082443    0.14196405    0.00000000
     atom    3 type  1   force =    -0.50847780    0.10558208    0.00000000
     atom    4 type  1   force =     0.75704277   -0.17646111    0.00000000

     Total force =     0.989284     Total SCF correction =     0.000255
```

Forces on atoms are quite large.

We now optimize the structure by two ways:

A) damped molecular dynamics

B) BFGS minimization

PAY ATTENTION !
This number measures the error on forces given by a non perfect self-consistency.
It has to be much smaller than the force itself.
Connected to `conv_thr`.

Copy the input file for SCF to a new file, and open it with PWgui:

```
cp acetylene.scf.in acetylene.damp.in

pwgui
```

guido.fratesi@unimi.it

C_2H_2 damped dynamics

Modify the new input file `acetylene.damp.in`: use an editor, or PWgui to

1) Specify the following variables in the "Control" namelist:

```
   calculation  = "relax",
   dt           = 20.D0,
```

2) Set a stricter SCF threshold ("Electrons" namelist):

```
   conv_thr    = 1.D-8,
```

3) Add "Ions" namelist:

```
 &IONS
   ion_dynamics       = "damp",
   pot_extrapolation = "second_order",
   wfc_extrapolation = "second_order",
 /
```

(these extrapolations make the SCF loop shorter)

4) Set equal masses (we are not interested in a real dynamics!)

```
 H   1.0   H.US_PBE.RRKJ3.UPF
 C   1.0   C.US_PBE.RRKJ3.UPF
```

5) Save and run:

```
   pw.x < acetylene.damp.in > acetylene.damp.out
```

C_2H_2 damped dynamics

Examine the output:

1) Scroll the file:

`less acetylene.damp.out` (press q to exit)

2) Extract key quantities:

total energy: `grep ! acetylene.damp.out | nl`

total force: `grep "Total force" acetylene.damp.out | nl`

3) Use XCrySDen to visualize the dynamics:

`xcrysden --pwo acetylene.damp.out`

(remember to select "reduce dimension to 0D" and "Display All Coordinates as Animation"; type "f" to visualize the forces)

At convergence, forces are smaller the the specified (or default) threshold, and the algorithm stops:

```
     Forces acting on atoms (Ry/au):

     atom    1 type  2   force =    -0.00052921   -0.00029862    0.00000046
     atom    2 type  2   force =     0.00029473    0.00021132   -0.00000059
     atom    3 type  1   force =     0.00006651   -0.00020371   -0.00000019
     atom    4 type  1   force =     0.00016798    0.00029100    0.00000032

     Total force =     0.000539     Total SCF correction =     0.000021

     Damped Dynamics: convergence achieved in  17 steps
```

guido.fratesi@unimi.it

C_2H_2 BFGS minimization

1) Copy the input file for damped dynamics to a new file, and open it with PWgui:

```
cp acetylene.damp.in acetylene.bfgs.in
pwgui
```

2) In "Ions" namelist

change: `ion_dynamics = 'damp' ,`

to: `ion_dynamics = 'bfgs' ,`

3) Set a variable SCF threshold
(100 times more accurate closer to the minimum of energy):
In "Electrons" namelist

Change: `conv_thr = 1.D-8 ,`

To: `conv_thr = 1.D-6 ,`

In "Ions" namelist

Add: `upscale = 100 ,`

4) Run the calculation

```
pw.x < acetylene.bfgs.in > acetylene.bfgs.out
```

5) Look at the output

6) Compare final positions, energy, and number of steps with damped dynamics

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Structural optimization of a slab

We want now to optimize the geometry of an Al(001) slab.

1) Take a look at the provided input file for SCF calculation, al001.scf.in.
we have five atomic layers at the bulk-truncated positions (`alat` units):

```
Al      0.000000000    0.000000000    2.828426000    1  1  1
Al      0.500000000    0.500000000    2.121320000    1  1  1
Al      0.000000000    0.000000000    1.414213000    1  1  1
Al      0.500000000    0.500000000    0.707107000    0  0  0
Al      0.000000000    0.000000000    0.000000000    0  0  0
```

(The bottom two layers are fixed)
Visualize the structure with XCrySDen (show multiple unit cells, press **`shift-n`**)

2) Copy to a new file **`cp al001.scf.in al001.bfgs.in`**
and edit it by adding the variables for the structural optimization, as seen before.

4) Run the calculation **`pw.x < al001.bfgs.in > al001.bfgs.out`**

5) Look at the optimized geometries:

```
Al      -0.000000019  -0.000000008   2.757233372
Al       0.499999997   0.499999999   2.089582133
Al      -0.000000002  -0.000000001   1.397022977
Al       0.500000000   0.500000000   0.707107000
Al       0.000000000   0.000000000   0.000000000
```

6) Compare with experiments (LEED), but before check all the convergency parameters, which for this exercise are not accurate enough!