Example 3

Cupper (bulk & surface)

Pseudopotential generation

- Generate pseudopotential without PCC

  - pg.sh Cu.inp
  - cd Cu
  - gnuplot –persist pseudo.gplot
    pots.gplot
    charge.gplot

- Generate pseudopotential with PCC

  pg.sh Cu.pcc.inp

  - Check “Total pseudocore charge” in OUT
  - Plot pseudo, pots, charge

Pseudopotential test

- Open the Cu.test.inp file.
- Run the test

  - pt.sh Cu.test.inp Cu.pcc.vps
  - cd Cu.test-Cu.pcc
  - grep `&d´ OUT

The role of the Basis

- Directory Example-3/bulk-fcc/ contains input files to run bulk fcc-Cu with 3 different basis sets: SZ, SZP and DZP
- Run siesta for each basis and observe the differences in the bandstructure.

SUMMER SCHOOL ON COMPUTATIONAL MATERIALS SCIENCE

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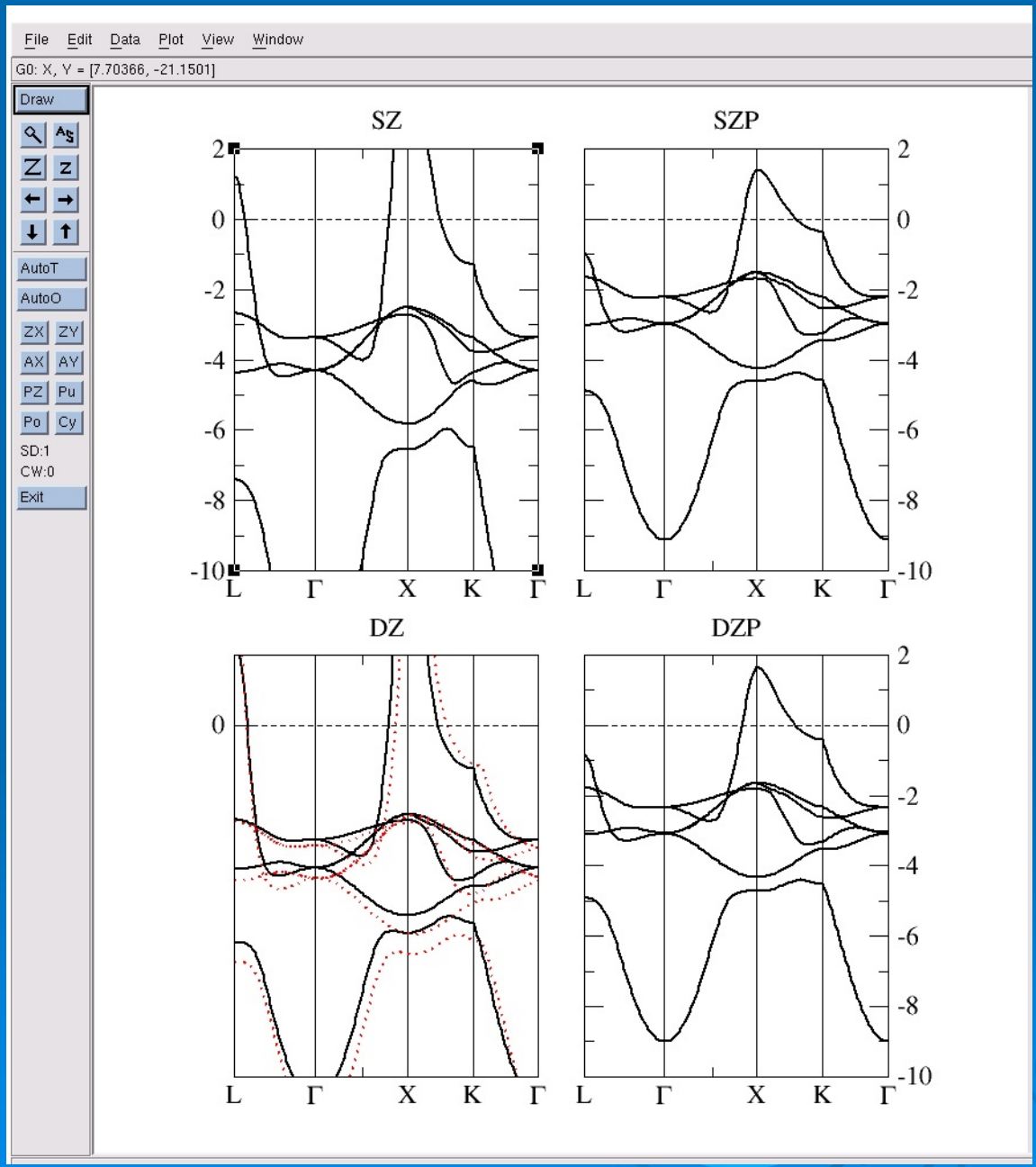
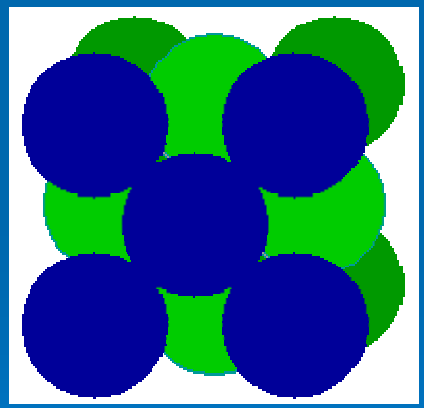
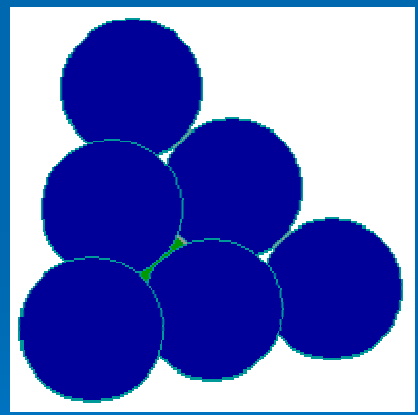


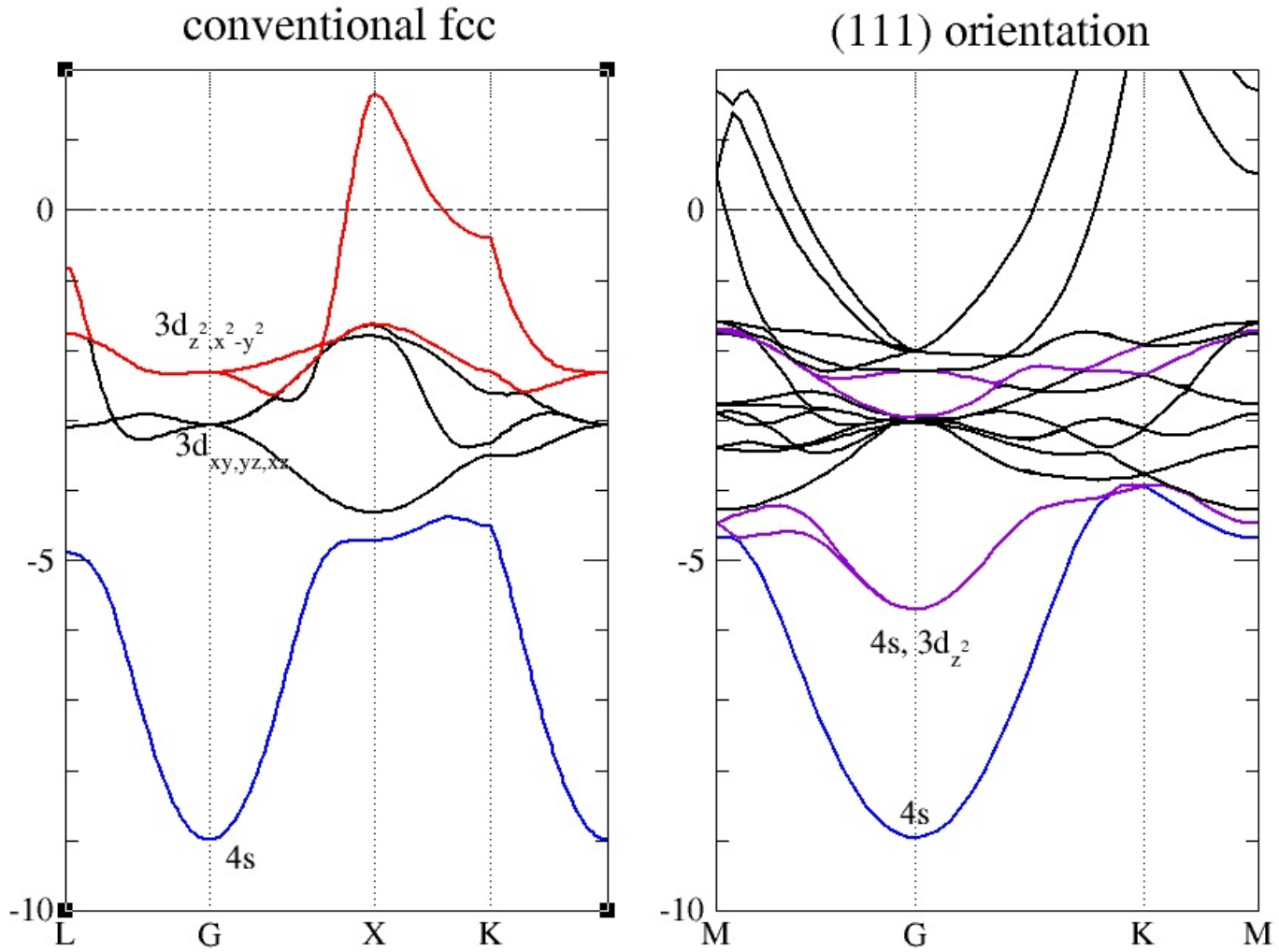
Bulk-111

- The directory SIESTA/Example-3/bulk-111 contains the input file for fcc-Cu with a different unit cell, in which the c-axis is along the (111) direction.





- Calculate the bandstructure for the new unit cell, and compare with that of the conventional fcc.


conventional fcc
(111) orientation
0
-5
-10
$3d_{z^2,x^2-y^2}$
$3d_{xy,yz,xz}$
4s
$4s, 3d_{z^2}$
L
G
X
K
M

Cu(111) surface

It is not always easy to achieve convergence (specially for metals!).

- Directory Example-3/surface-111/ contains input files to run surface of Cu-111. Try to converge the DM.

- If the run takes too long, try to use the saved DM file in the Converged/ subdirectory.

Cu(111) surface

- Plot the band structure for the converged surface.
- Cu(111) has a surface state that can be easily seen in a gap of the projection of the bulk bands in the 2D Brillouin-zone.
- Use the utility readwf to check the contributions of the atomic orbitals to the bands near the Fermi level at the Γ-point. Notice that the surface states only have contributions comming from atoms close to the surface of the slab.

File Edit Data Plot View Window

G4: X, Y = [2.38305, -5.33769]

Draw

AutoT

AutoO

ZX ZY

AX AY

PZ Pu

Po Cy

SD:1

CW:0

Exit

9 layers 12 layers 15 layers 18 layers 21 layers

4 2 0 -2 -4 -6 -8 -10

M Γ K M Γ K M Γ K M Γ K M Γ K