Dipole Corrections and workfunction

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Below you will find plots of the laterally averaged electrostatic potential of a 2 layer Al slab with a Na atom on one side of it, similar in spirit to the work in the original dipole correction reference [1][1]. You should also see a followup correction to Neugebauer's work by Lennart Bengtsson [2], as this is implemented in the DipoleCorrection used in Dacapo. The scripts can be found in an appendix at the end.

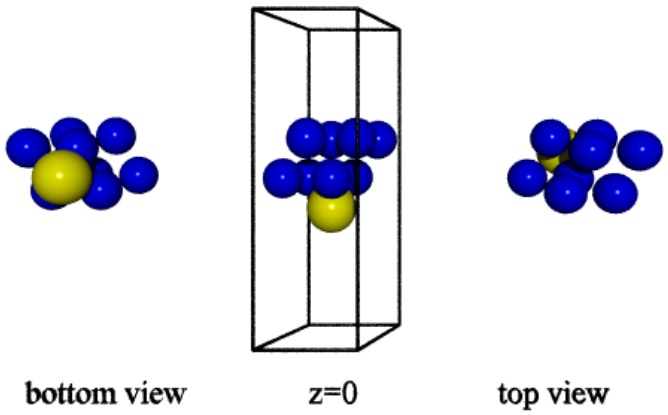

Figure 1: Slab geometry

[1]These are very crude calculations, the slabs are very thin, not relaxed and only a single k-point is used. They only show the effect of the dipole correction, and are used to show how to analyze the effects in the new ASE environment.

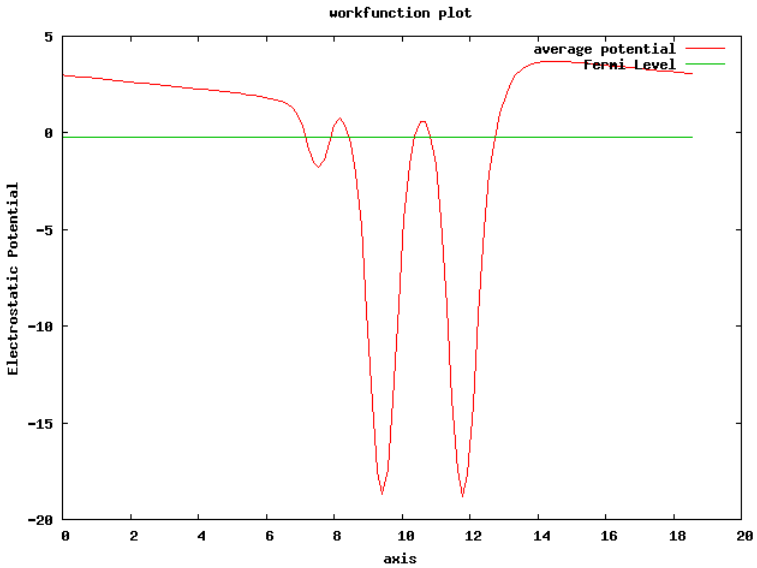

Figure 2: No Dipole correction defined. You see that the vacuum level potential is not well-defined, which makes interpreting the work function difficult.

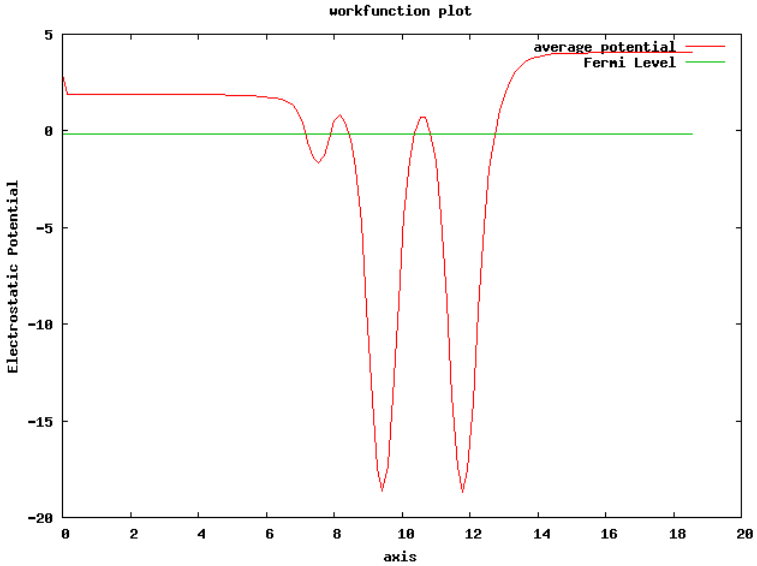

Figure 3: Dipole correction turned on. Note the jump in potential near z=0, and that now the vacuum levels are well defined. Also, there are now 2 well-defined work functions, one for the side with Na on it (Na is near z=7) with a value of about 2 eV and one for the bare side of the slab (z ¿ than about 13) of about 4 eV (you can calculate this exactly by subtracting the Fermi level from the vacuum potential). Compare this to the last line of the output in the txt file by grepping for DIP, shown below. Here, Work_f1 corresponds to the bare slab side, and Work_f2 corresponds to the Na slab side. You get the same result if the slab is not centered, see Figure 4

```
 FILE_IO: Writing netCDF formatted output to file Alslab_Na_DIP.nc
 DIP: Z_0 [A]    0.000000 nzzero:   1 119 120   2   3
 DIP:
 DIP:   u_damp       u    Field_1  Field_2  Work_f1  Work_f2  V_jump   E_dip
 DIP:     [eA]     [eA]    [V/A]    [V/A]     [eV]     [eV]     [V]     [eV]
.
.
.
 DIP:    -0.340   -0.341   -0.001    0.000    4.185    2.022   -2.164   -3.050
 DIP:    -0.340   -0.341   -0.001    0.000    4.186    2.022   -2.166   -3.053
 DIP:    -0.340   -0.341   -0.001    0.000    4.187    2.020   -2.167   -3.054
 DIP:    -0.340   -0.341   -0.001    0.000    4.187    2.020   -2.168   -3.055
 DIP:    -0.340   -0.341   -0.001    0.000    4.188    2.019   -2.169   -3.056
```

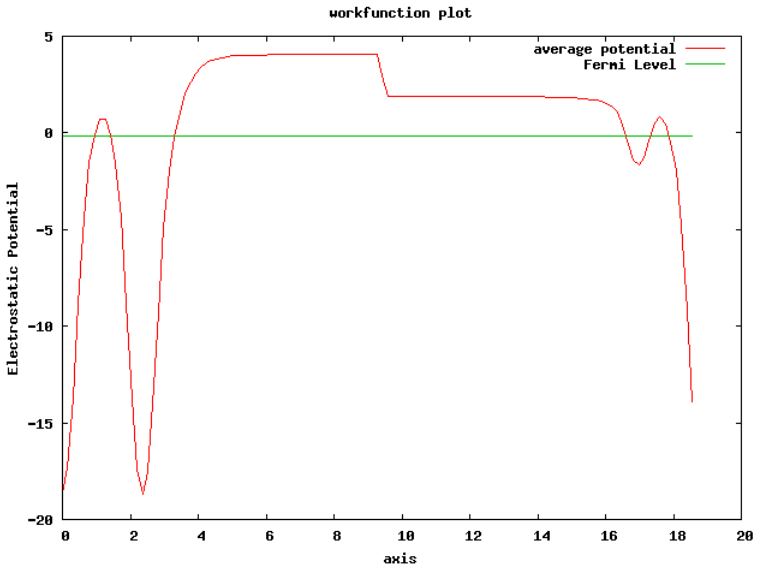

Figure 4: Averaged potential for a slab not centered in the unit cell.. Note the very prominent jump in potential in the middle of the slab, this is the Dipole Correction.

```
grep DIP Alslab_Na_DIP_0.txt
 FILE_IO: Writing netCDF formatted output to file Alslab_Na_DIP_0.nc
 DIP: Z_0 [A]    9.353074 nzzero:  61  59  60  62  63
 DIP:
 DIP:   u_damp       u    Field_1  Field_2  Work_f1  Work_f2  V_jump   E_dip
 DIP:     [eA]     [eA]    [V/A]    [V/A]     [eV]     [eV]     [V]     [eV]
.
.
.
 DIP:    -0.339   -0.339    0.000    0.001    4.185    2.022   -2.162   -3.047
 DIP:    -0.339   -0.340   -0.001    0.000    4.185    2.023   -2.162   -3.047
 DIP:    -0.340   -0.340   -0.001    0.000    4.185    2.023   -2.163   -3.048
 DIP:    -0.340   -0.341   -0.001    0.000    4.185    2.022   -2.164   -3.050
 DIP:    -0.340   -0.341   -0.001    0.000    4.186    2.022   -2.166   -3.053
 DIP:    -0.340   -0.341   -0.001    0.000    4.187    2.020   -2.167   -3.054
 DIP:    -0.340   -0.341   -0.001    0.000    4.187    2.020   -2.168   -3.055
 DIP:    -0.340   -0.341   -0.001    0.000    4.188    2.019   -2.169   -3.056
```

A scripts

A.1 Using dipole correction

```
#!/usr/bin/env python
from Dacapo import Dacapo
from ASE import Atom,ListOfAtoms

# setup the static Al slab
alslab =  ListOfAtoms([Atom('Na',(.33,.16,-.1)),
                       Atom('Al',(0, 0, 0)),
                       Atom('Al',(0, 0.5, 0)),
                       Atom('Al',(0.5, 0, 0)),
                       Atom('Al',(0.5, 0.5, 0)),
                       Atom('Al',(0.3333333, 0.166666667, 0.125)),
                       Atom('Al',(0.3333333, 0.666666667, 0.125)),
                       Atom('Al',(0.8333333, 0.166666667, 0.125)),
                       Atom('Al',(0.8333333, 0.666666667, 0.125))])

# translating the atoms to the center of the cell makes the potential plots look nicer
for atom in alslab:
    atom.SetCartesianPosition(atom.GetCartesianPosition() + (0,0,0.5))

unitcell = [[5.72756492761103, 0, 0],
            [-2.86378246380552, 4.96021672913593, 0],
            [0,0,18.7061487217439]]

alslab.SetUnitCell(unitcell)

calc = Dacapo(planewavecutoff = 340,
              nbands = 30)
calc.DipoleCorrection()
calc.SetNetCDFFile('Alslab_Na_DIP.nc')
alslab.SetCalculator(calc)

energy = alslab.GetPotentialEnergy()
```

A.2 Plotting average potential

```
#!/usr/bin/env python
from Dacapo import Dacapo
import Gnuplot,Numeric

atoms = Dacapo.ReadAtoms('Alslab_Na_DIP_0.nc')
```

```
calc = atoms.GetCalculator()

### should the calculator method return this grid?
from ASE.Utilities.Grid import Grid
from ASE.Utilities import Vector,VectorSpaces
pot = Grid(calc.GetElectrostaticPotential(),
           space=VectorSpaces.BravaisLattice(atoms.GetUnitCell()))

avg_pot = pot.GetAverageAlongAxis(2)

E_f=calc.GetFermilevel()

# define the z-axis for plotting, in real units
Number_of_points=len(avg_pot)
end_point=Vector.Vector(pot.GetSpace().GetBasis()[2]).Length()
step=end_point/float(Number_of_points-1)
axis=Numeric.arange(0,end_point,step)

###create a line with value of the fermi energy
E_f_data=[E_f]*len(avg_pot)

gplot=Gnuplot.Gnuplot(persist=1)
gplot.xlabel('axis')
gplot.ylabel('Electrostatic Potential')
gplot.title('workfunction plot')
d1=Gnuplot.Data(zip(axis,avg_pot),title="average potential",with='lines')
d2=Gnuplot.Data(zip(axis,E_f_data),title="Fermi Level",with='lines')
gplot.plot(d1,d2)

gplot('set terminal png')
gplot('set output "dip_z=0.png"')
gplot.replot()

### print data for reading
for tuple in zip(axis,avg_pot-E_f): print tuple
```

References

[1] J. Neugebauer and M. Scheffler. Adsorbate-substrate and adsorbate-adsorbate interactions of Na and K adlayers on Al(111). *Phys. Rev. B*, 46:16067, 1992.

[2] L. Bengtsson. Dipole correction for surface supercell calculations. *Phys. Rev. B*, 59(19):12301–12304, 1999.