Tutorial 2

I. The INCAR file

Input: I INCAR

- VASP basically uses 4 input files for standard production runs
- INCAR: gives the input parameters which steer the calculation:
- The default values set by VASP itself are a clever choice to do standard calculations
- these standard settings can be modified to specify:
  - what do you want to do? (scf calculation, DOS, dielectric properties ...)
  - give some the basic inputs concerning the required precision, the requested convergence, clever guesses for the input to speed up the convergence ...)

II. The POSCAR file

Input II: POSCAR

```
fcc:  Ni
3.53
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
Ni
1
Selective Dyn
Cartesian
0 0 0 ( T T T)
```

Geometry Input

- header (comment)
- overall scaling constant
- 3-6: Bravais Matrix
- name(s) of the atom(s)
- number of the atoms (of each atom type)
- (optional: selective dynamics)
- Carthesian | Direct
- positions of the atoms

III. The KPOINTS file

Input: III KPOINTS

```
Automatic mesh
0
G (M)
4 4 4
0.  0.  0.
```

general format for scf runs...

1. header (comment)
2. $N_{\vec{k}} = 0$: automatic generation scheme
3. Γ-centered (MP) grid
4. # of subdivisions N_i along b_i
5. optional shift of the mesh (s_i)

IV. The POTCAR file

Input: IV POTCAR

- description of the PP
  - data that were required for generating the PP
  - number of valence electrons
  - atomic mass
  - energy cutoff
- if the cell contains different atoms, the atomic POTCARs have to be concatenated, in the same order as the atoms are given in POSCAR
- different XC-types must not be mixed

Output files

OUTCAR

- detailled output of a VASP run, including
  - summary of the input parameters set
  - information about the electronic steps: E_{Fermi}, KS-eigenvalues
  - stress tensors
  - forces on the atoms of each calculation
  - local charges, magnetic moments
  - dielectric properties
- the amount of output written onto OUTCAR can be chosen by setting `NWRITE` in INCAR

OSZICAR, job.stdout

- gives a short summary of the results
- chosen scf-algorithm
- convergence of the E, charge- and spin densities
- free energies, magnetic moments of the cell

Output files

CONTCAR, XDATCAR

- CONTCAR: updated geometry data *at the end of a run*
  - lattice parameter
  - Bravais matrix
  - ionic positons
  - (velocities)
- the format of CONTCAR is the same as for POSCAR, $\Rightarrow$ it can be used directly for continuation runs after havine been copied to POSCAR)
- XDATCAR: updated ionic positions of each ionic step

DOSCAR,CHGCAR,WAVECAR

- DOSCAR: total DOS and integrated DOS, (local partial DOS)
- CHGCAR: charges (ρ * V)
- WAVECAR wavefunction coefficients. WAVECAR can eg be used to continue from a previous run.

Documentation

- The VASP manual (http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html)

  Index: http://cms.mpi.univie.ac.at/vasp/vasp/Index.html

- The VASP wiki (http://cms.mpi.univie.ac.at/wiki/index.php/Main_page)

  INCAR-tags: http://cms.mpi.univie.ac.at/wiki/index.php/Category:INCAR

A bit of surface science

Examples:

- Ni(100)
  surface relaxation
  surface energy
  LDOS
  surface bandstructure

- Ni(111)
  clean surface
  CO adsorption
  LDOS
  workfunction (change)
  frequencies

- STM of graphite and graphene

Ni(100) surface relaxation (Example: 3_1_Ni100clean_rel)

```
 fcc (100) surface
 3.53
   .50000   .50000   .00000
  -.50000   .50000   .00000
   .00000   .00000  5.00000
  5
Selective Dynamics
Cartesian
   .00000   .00000   .00000 F F F
   .00000   .50000   .50000 F F F
   .00000   .00000  1.00000 F F F
   .00000   .50000  1.50000 T T T
   .00000   .00000  2.00000 T T T
```

POSCAR

- Ni lattice constant 3.53 Å
- 1 atom per layer $\Rightarrow p(1 \times 1)$ cell
- 5 nickel layers
- first two layers (of one side) relaxed
- $3 \cdot 3.53 = 10.59$Å vacuum

POTCAR

PAW-GGA potential for Ni

Ni(100) surface relaxation (Example: 3_1_Ni100clean_rel)

```
general:
  SYSTEM = clean Ni(100) surface
  ISTART = 0 ; ICHARG=2
  ENCUT  =    270
  ISMEAR =    2  ; SIGMA = 0.2
spin:
  ISPIN=2
  MAGMOM = 5*1
dynamic:
  IBRION = 1
  NSW    = 100
  POTIM = 0.2
```

```
K-Points
 0
Monkhorst-Pack
9 9 1
0 0 0
```

INCAR

- startjob; initial charge-density from overlapping atoms
- energy cut-off: 270 eV (default)
- MP-smearing (metal!)
- spinpolarized calculation initial moments of 1
- ionic relaxation

KPOINTS

- equally spaced mesh
- odd $\rightarrow$ centered on Γ
- results in 15 k-points in IBZ
- 1 in z-direction !

Ni(100) surface relaxation (Example: 3_1_Ni100clean_rel)

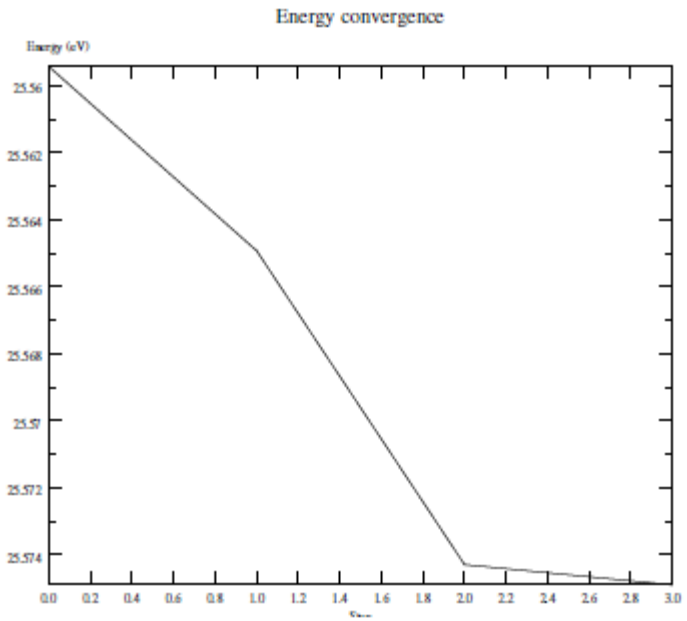
forces in the first and last step (in OUTCAR)

```
POSITION                                       TOTAL-FORCE (eV/Angst)
-----------------------------------------------------------------------------------
     0.00000      0.00000      0.00000         0.000000      0.000000      0.391352
     0.00000      1.76500      1.76500         0.000000      0.000000     -0.397024
     0.00000      0.00000      3.53000         0.000000      0.000000      0.005117
     0.00000      1.76500      5.29500         0.000000      0.000000      0.391161
     0.00000      0.00000      7.06000         0.000000      0.000000     -0.390607
-----------------------------------------------------------------------------------
   total drift:                                 0.000000      0.000000      0.016391

POSITION                                       TOTAL-FORCE (eV/Angst)
-----------------------------------------------------------------------------------
     0.00000      0.00000      0.00000         0.000000      0.000000      0.399012
     0.00000      1.76500      1.76500         0.000000      0.000000     -0.377003
     0.00000      0.00000      3.53000         0.000000      0.000000      0.105799
     0.00000      1.76500      5.32685         0.000000      0.000000     -0.062054
     0.00000      0.00000      7.02377         0.000000      0.000000     -0.065753
-----------------------------------------------------------------------------------
   total drift:                                 0.000000      0.000000     -0.042925
```

Ni(100) surface relaxation (Example: 3_1_Ni100clean_rel)

- energy changes during relaxation
  from -25.556 to -25.571 eV
  $\Rightarrow$ relaxation energy $E^{\text{rel}} = -15$ meV
- surface energy of (unrelaxed) surface according
  $$\boxed{\sigma = \frac{1}{2}(E_{\text{surf}} - N_{\text{atoms}} \cdot E_{\text{bulk}})}$$
  $\Rightarrow \sigma^{\text{unrel}} = \frac{1}{2}(-25.556 - 5 \cdot (-5.457)) = 0.86$ eV
- $\sigma = \sigma^{\text{unrel}} + E^{\text{rel}} = 0.84$ eV

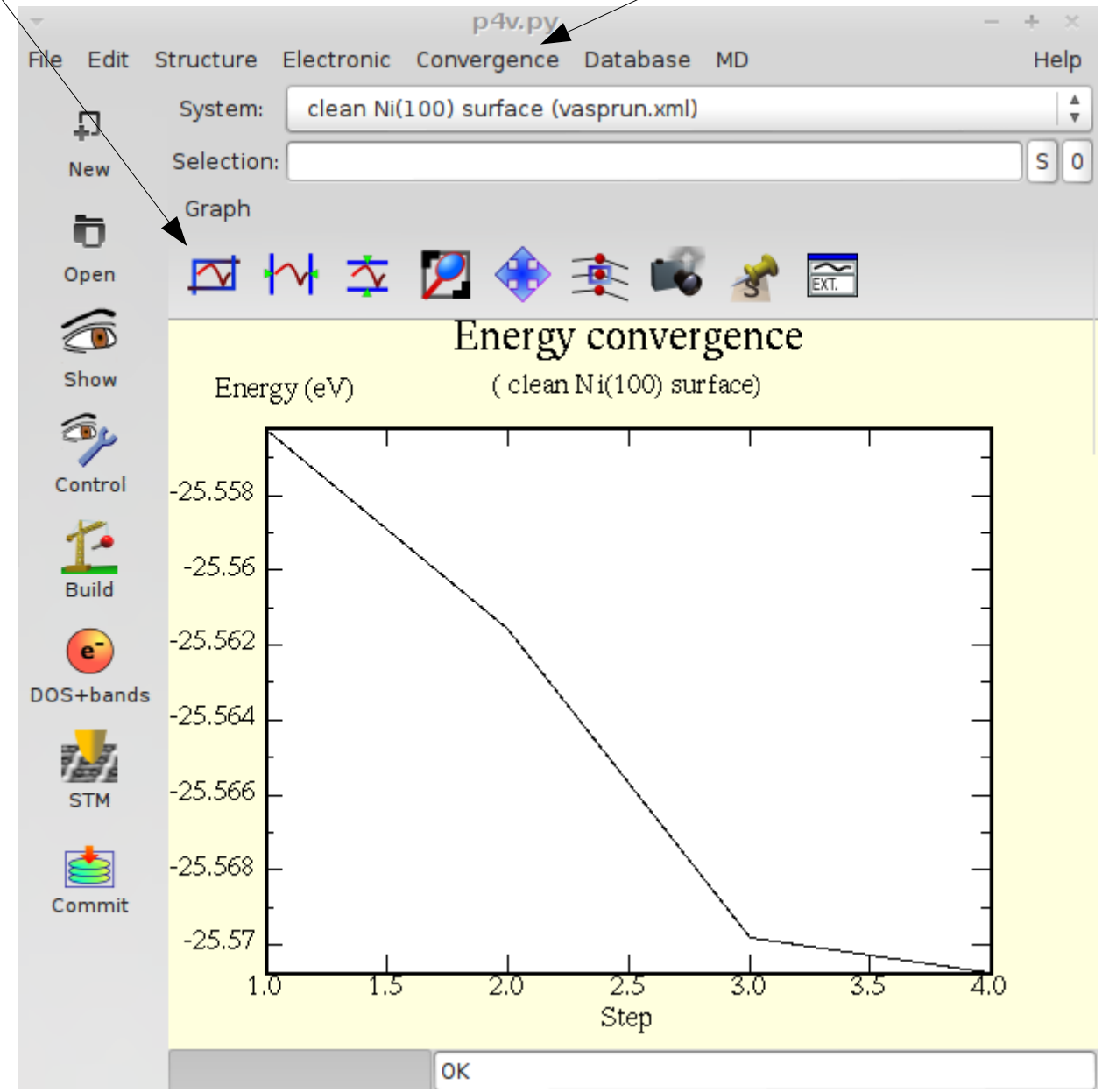


N.B.: The setup for the calculation of the “bulk” energy, you'll find in the *3_1_Ni100clean_rel/bulk* subdirectory

Ni(100) surface relaxation (Example: 3_1_Ni100clean_rel)

“Update” graph

Go to “Convergence/Energy”



Ni(100) surface relaxation (Example: 3_1_Ni100clean_rel)

Final geometry (from CONTCAR or OUTCAR file):

```
fcc (100) surface
   3.53000000000000
     0.5000000000000000    0.5000000000000000    0.0000000000000000
    -0.5000000000000000    0.5000000000000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000    5.0000000000000000
   Ni
     5
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.5000000000000000  0.5000000000000000  0.1000000000000014   F   F   F
  0.0000000000000000  0.0000000000000000  0.2000000000000028   F   F   F
  0.5000000000000000  0.5000000000000000  0.3018043743226639   T   T   T
  0.0000000000000000  0.0000000000000000  0.3979474020596729   T   T   T
```

- inward relaxation of surface layers

$$\Rightarrow \Delta d_{12} = ((0.3979 - 0.3018) - 0.1)/0.1 * 100 = -3.9\%$$

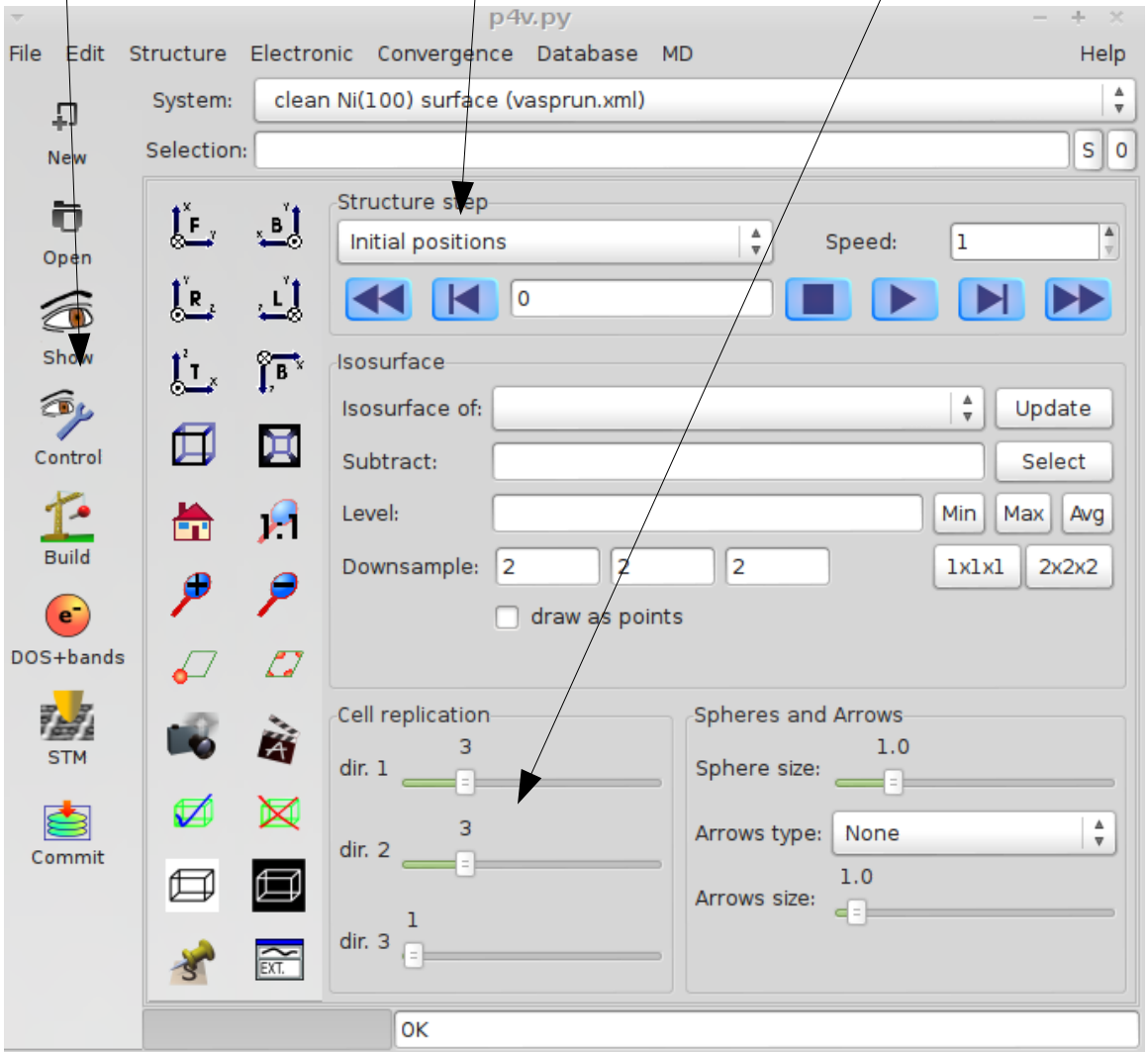
$$\Rightarrow \Delta d_{12} = ((0.3018 - 0.2000) - 0.1)/0.1 * 100 = +1.8\%$$

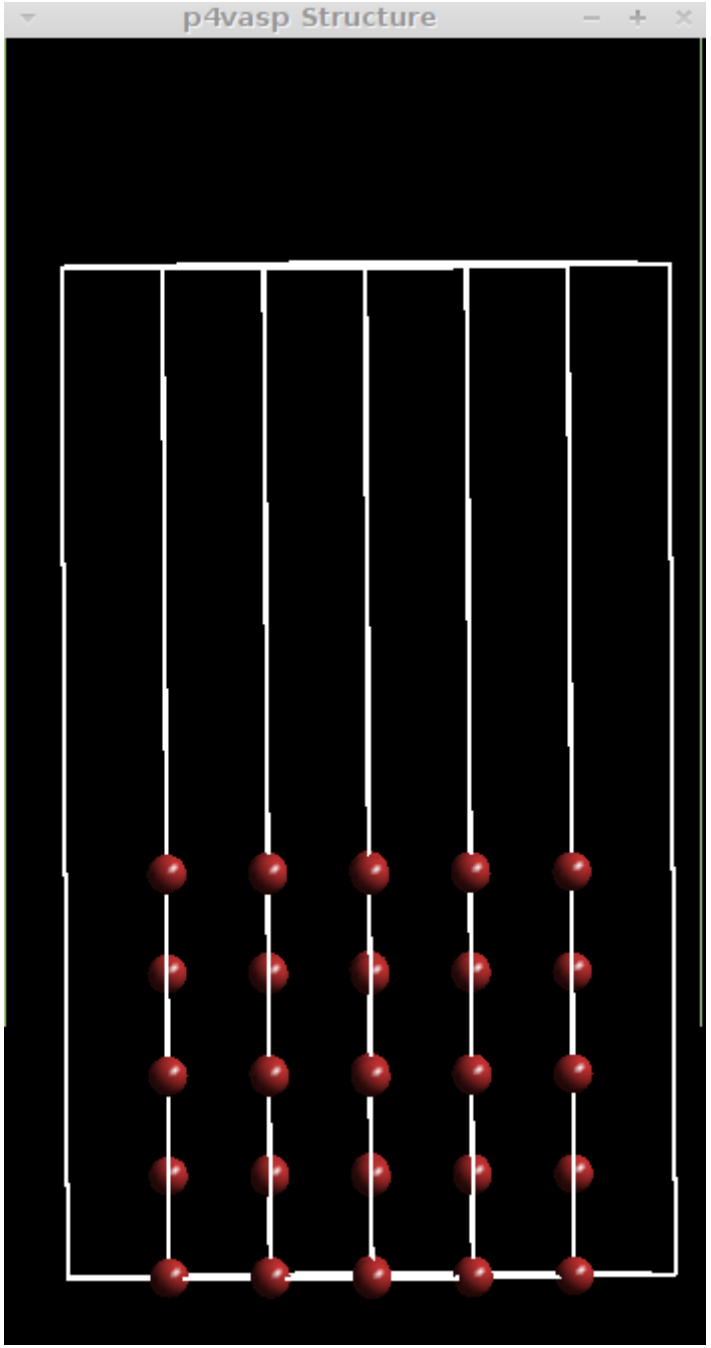
Ni(100) surface relaxation (Example: 3_1_Ni100clean_rel)

Go to “Control”

Possibly replicate cells

Select “intial” or “final” positions





Ni(100) LDOS (Example: 3_2_Ni100clean_LDOS)

```
general:
   SYSTEM = clean (100) Ni surface
   ENMAX = 270
   ISMEAR =   -5
   ALGO= Normal

spin:
   ISPIN=2
   MAGMOM = 5*1

   LORBIT = 11
```

INCAR

- tetrahedron method
- LM and site decomposed DOS

N.B.: We want to use the optimized structure of 3_1_Ni100clean_rel:

Normally this would mean copying the CONTCAR of 3_1_Ni100clean_rel to POSCAR in the directory where you want to run 3_2_Ni100clean_LDOS.

In this case, however, that has already been taken care of, andthe POSCAR file in 3_2_Ni100clean_LDOS is already the correct one.

Ni(100) LDOS (Example: 3_2_Ni100clean_LDOS)

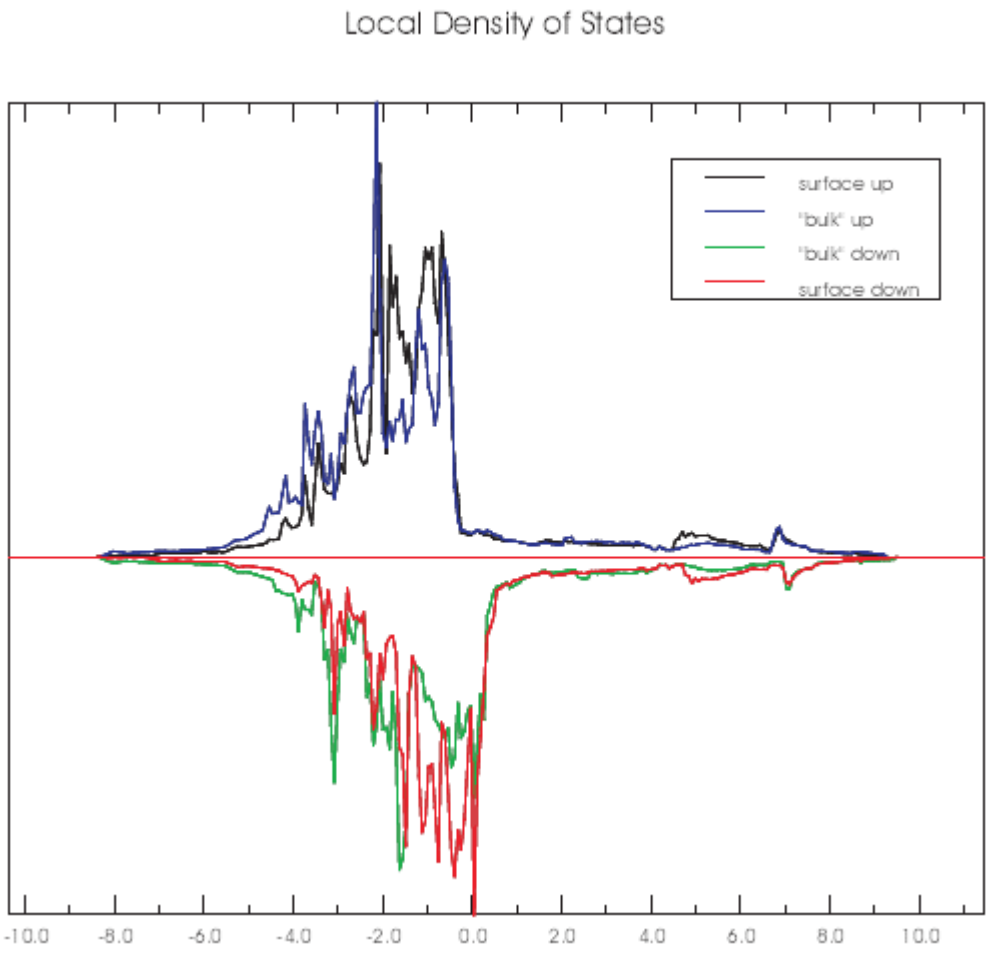
```
 total charge
# of ion      s        p        d        tot
----------------------------------------
  1         0.461    0.316    8.331    9.108
  2         0.483    0.466    8.323    9.273
  3         0.484    0.462    8.324    9.270
  4         0.490    0.481    8.329    9.300
  5         0.472    0.337    8.341    9.150
----------------------------------------------
tot         2.390    2.062   41.648   46.100

 magnetization (x)
# of ion      s        p        d        tot
----------------------------------------
  1        -0.003   -0.019    0.715    0.692
  2        -0.008   -0.023    0.619    0.588
  3        -0.007   -0.024    0.620    0.589
  4        -0.008   -0.024    0.622    0.591
  5        -0.004   -0.020    0.705    0.681
----------------------------------------------
tot        -0.030   -0.110    3.281    3.141
```

- at the end of the OUTCAR file information on local charge and magnetization is given
- using `LORBIT = 1` and changing `RWIGS` the total number of electrons within the spheres could be adapted (nickel pseudopotential has a valence of 10)
- enhancement of the magnetic moment at the surface
- in the center “bulk like

Ni(100) LDOS (Example: 3_2_Ni100clean_LDOS)

- projection onto surface layer and bulk layer
- each spin component is plotted separately
- band narrowing at surface
- exchange splitting larger at surface

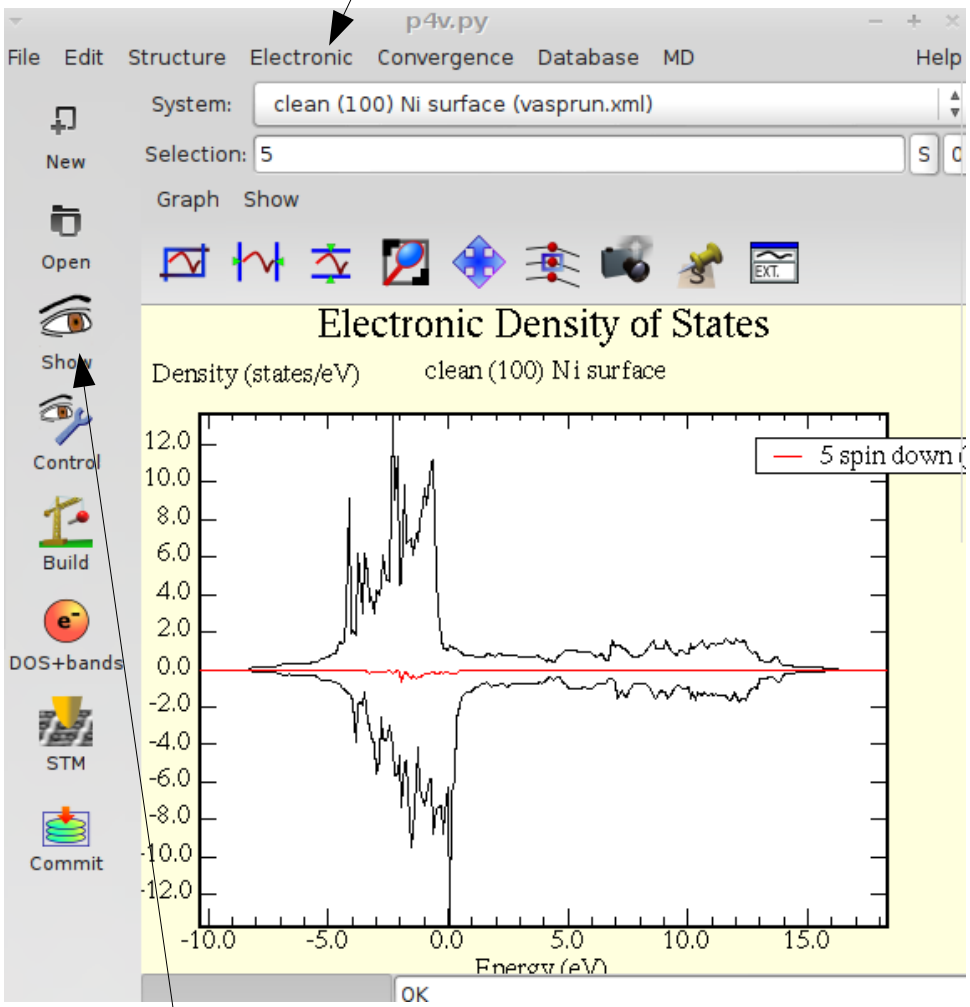


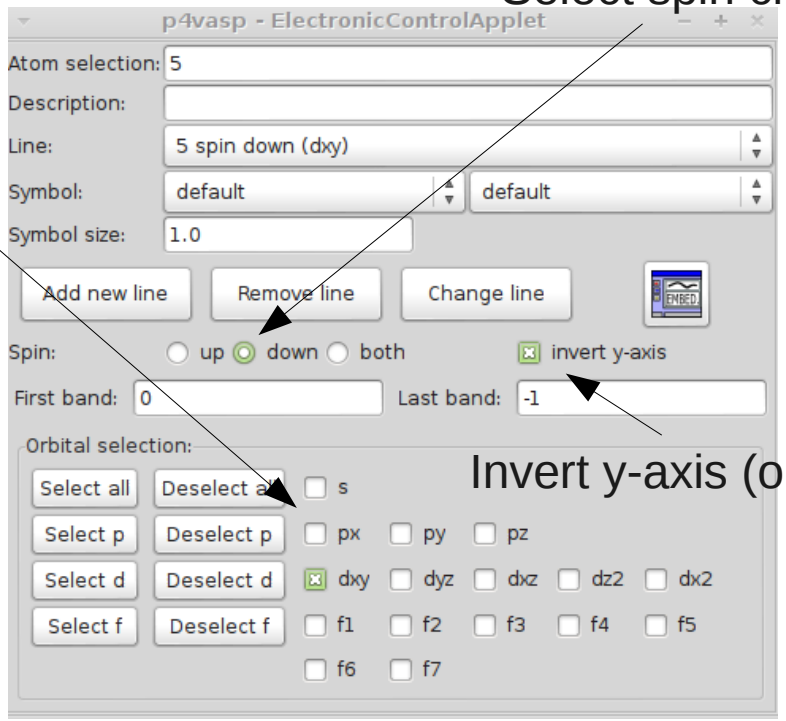
Ni(100) LDOS (Example: 3_2_Ni100clean_LDOS)

Select “Electronic/local DOS+bands control”

Select spin channel

Select orbital character

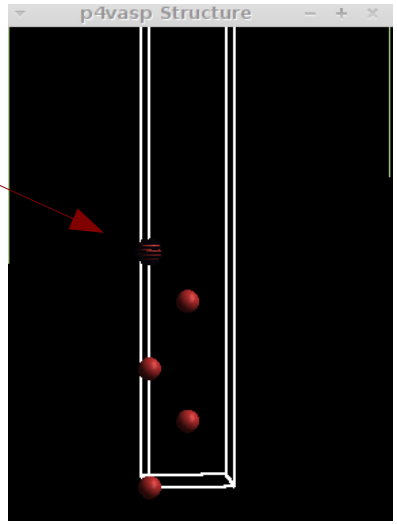




Invert y-axis (optional)

Place pointer over atom, and press space to select/deselect.

The selection should appear in the Electronic Control applet above



Press “Show” to show structure

Ni(100) surface bandstructure (Example: 3_3_Ni100clean_band)

```
  ICHARG = 11
general:
  SYSTEM = clean (100) nickel surface
  ENMAX  = 270
  ISMEAR =   2 ; SIGMA = 0.2
  ALGO= Normal

spin:
  ISPIN=2
  MAGMOM = 5*1

  LORBIT = 11
```

INCAR

- `ICHARG = 11`: read in charge density (1) and do not update it (+10) ⇒ non-selfconsistent run!

N.B.: You need to copy the CHGCAR file of example 3_2_Ni100clean_LDOS
Into the directory where you want to run 3_3_Ni100clean_band

Ni(100) surface bandstructure (Example: 3_3_Ni100clean_band)

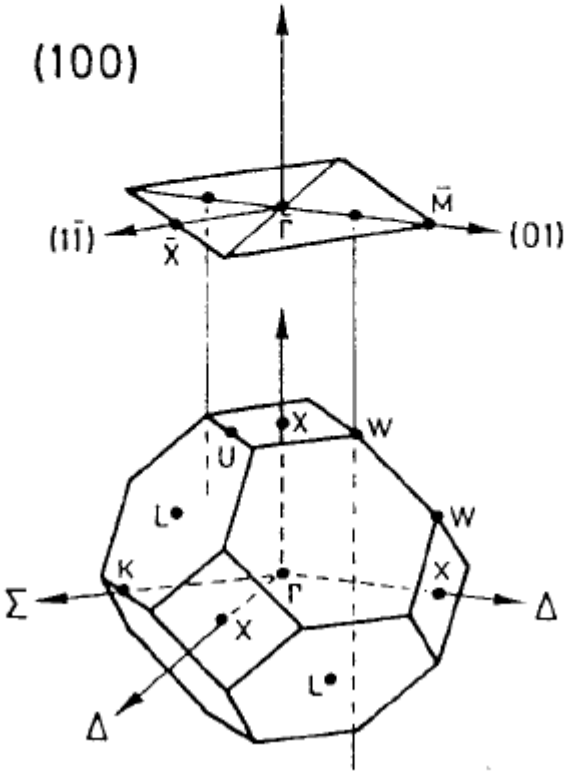
```
kpoints for band-structure G-X-M-G
  13
reziprok
   .00000   .00000   .00000    1
   .12500   .00000   .00000    1
   .25000   .00000   .00000    1
   .37500   .00000   .00000    1
   .50000   .00000   .00000    1

   .50000   .12500   .00000    1
   .50000   .25000   .00000    1
   .50000   .37500   .00000    1
   .50000   .50000   .00000    1

   .37500   .37500   .00000    1
   .25000   .25000   .00000    1
   .12500   .12500   .00000    1
   .00000   .00000   .00000    1
```

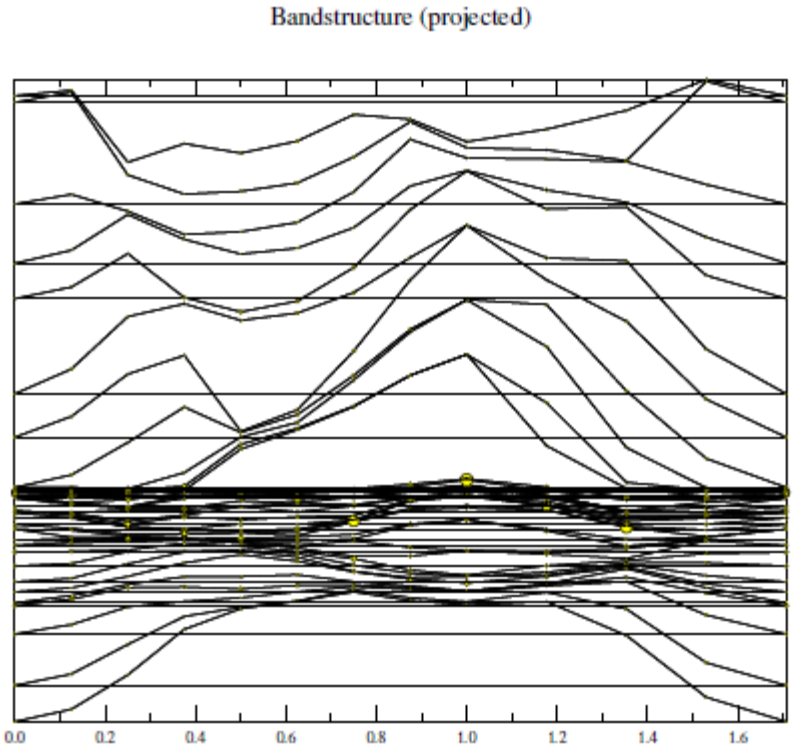
KPOINTS

- 13 k-points along line $\bar{\Gamma} - \bar{X} - \bar{M} - \bar{\Gamma}$
- in reciprocal coordinates
- all points with weight 1



Ni(100) surface bandstructure (Example: 3_3_Ni100clean_band)

```
...
Static calculation
charge density remains constant during run
spin polarized calculation
...
```



- in OUTCAR status message on actual job
  $\Rightarrow$ non-selfconsistent calculation

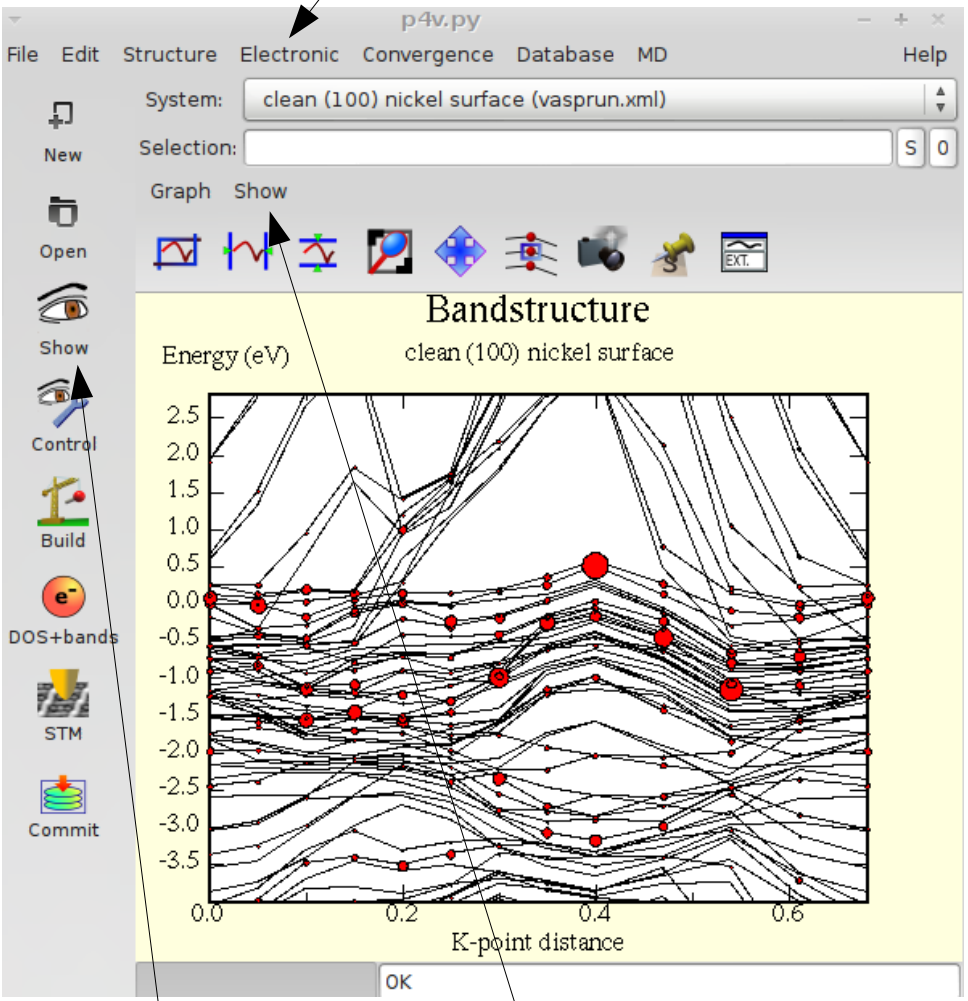
- bandstructure consists mainly out of bulk-like bands
- dots mark localization at surface layer

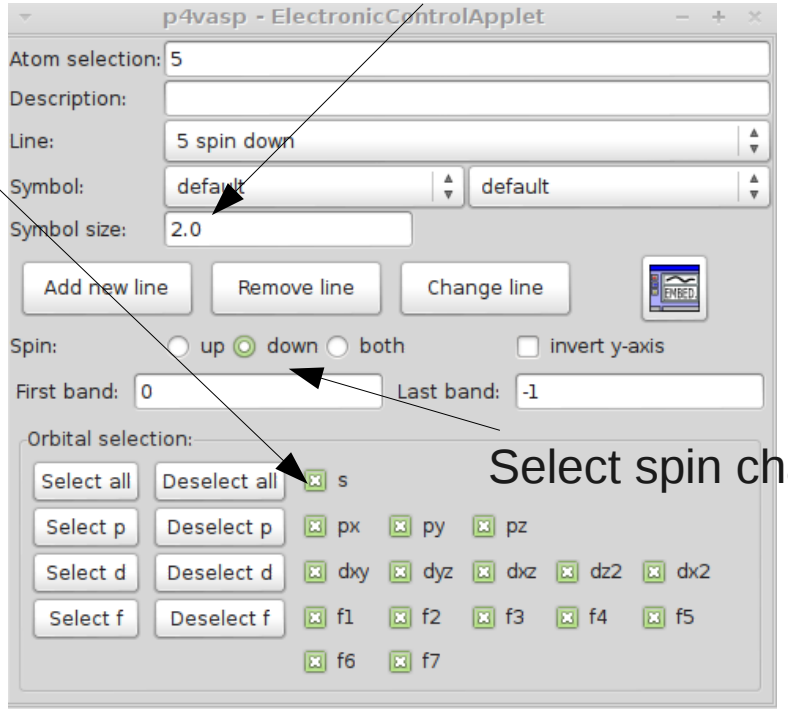
Ni(100) surface bandstructure (Example: 3_3_Ni100clean_band)

Select “Electronic/local DOS+bands control”

Choose symbol size

Select orbital character

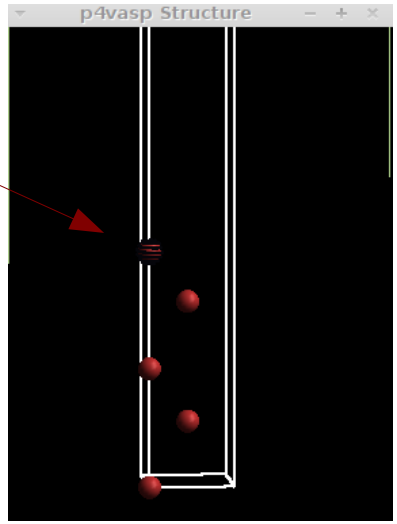




Select spin channel

Place pointer over atom, and press space to select/deselect.

The selection should appear in the Electronic Control applet above



Select “Bands”

Press “Show” to show structure

Ni(111) surface relaxation (Example: 3_4_Ni111clean_rel)

```
general:
  ISTART = 0;   ICHARG = 2
  SYSTEM = clean (111) surface
  ENMAX  = 270
  ISMEAR =    2  ; SIGMA = 0.2
  ALGO= Fast

dynamic:
  NSW=100
  POTIM = 0.2
  IBRION = 1
```

INCAR

- same INCAR file as previously for (100) surface
- spin-polarization neglected

Ni(111) surface relaxation (Example: 3_4_Ni111clean_rel)

```
 Ni - (111)
  3.53
   .70710678  .0000000  .000000
 -0.35355339 0.6123724  .000000
   .000000    .000000  5.196152
    5
selective dynamics
direct
.00000000 .00000000 .00000000  F  F  F
.33333333 .66666667 .11111111  F  F  F
.66666667 .33333333 .22222222  F  F  F
.00000000 .00000000 .33333333  T  T  T
.33333333 .66666667 .44444444  T  T  T
```

POSCAR

- similar setup as for (100) surface
- again 5 layers, 2 relaxed
- $(1 - .444) \cdot 5.196 \cdot 3.53 =$
  ~ 10.2Å of vacuum

Ni(111) surface relaxation (Example: 3_4_Ni111clean_rel)

Geometry and surface energy:

```
POSITION                                      TOTAL-FORCE (eV/Angst)
-----------------------------------------------------------------------------------
     0.00000      0.00000      0.00000         0.000000      0.000000      0.178848
     0.00000      1.44112      2.03805         0.000000      0.000000     -0.060127
     1.24804      0.72056      4.07609         0.000000      0.000000      0.004418
     0.00000      0.00000      6.11522         0.000000      0.000000      0.036384
     0.00000      1.44112      8.14905         0.000000      0.000000     -0.159523
-----------------------------------------------------------------------------------
   total drift:                                -0.000084      0.000107     -0.017457
```

- forces already at the beginning rather small
  $\Rightarrow$ small relaxations for compact surfaces
- for surface energy non-spin-polarized bulk nickel as reference !
  $\Rightarrow \sigma^{\text{unrel}} = \frac{1}{2}(-25.731 - 5 \cdot (-5.407)) = 0.65$ eV
  $\Rightarrow$ (111) surface more stable than (100) surface

N.B.: The setup for the calculation of the “bulk” energy, you'll find in the *3_4_Ni111clean_rel/bulk* subdirectory

CO@Ni(111) (Example: 3_5_COonNi111_rel)

```
 Ni - (111)
  3.53
   .70710678  .0000000  .000000
 -0.35355339 0.6123724  .000000
   .000000    .000000  5.1961524
    5 1 1
selective dynamics direct
.00000000 .00000000 .00000000  F  F  F
.33333333 .66666667 .11111111  F  F  F
.66666667 .33333333 .22222222  F  F  F
.00000000 .00000000 .33333333  T  T  T
.33333333 .66666667 .44444444  T  T  T
.33333333 .66666667 .54029062  T  T  T
.33333333 .66666667 .60298866  T  T  T
```

POSCAR

- two additional types (C+O)
  $\Rightarrow$ POTCAR!
- CO molecule put above surface atom
  $\Rightarrow$*on-top*
- $z_C = (.540 - .444) \cdot 5.196 \cdot 3.53 =$
  ~ 1.76Å
- $d_{CO} = (.603 - .540) \cdot 5.196 \cdot 3.53 =$
  ~ 1.16Å

POTCAR

- append carbon and oxygen potentials

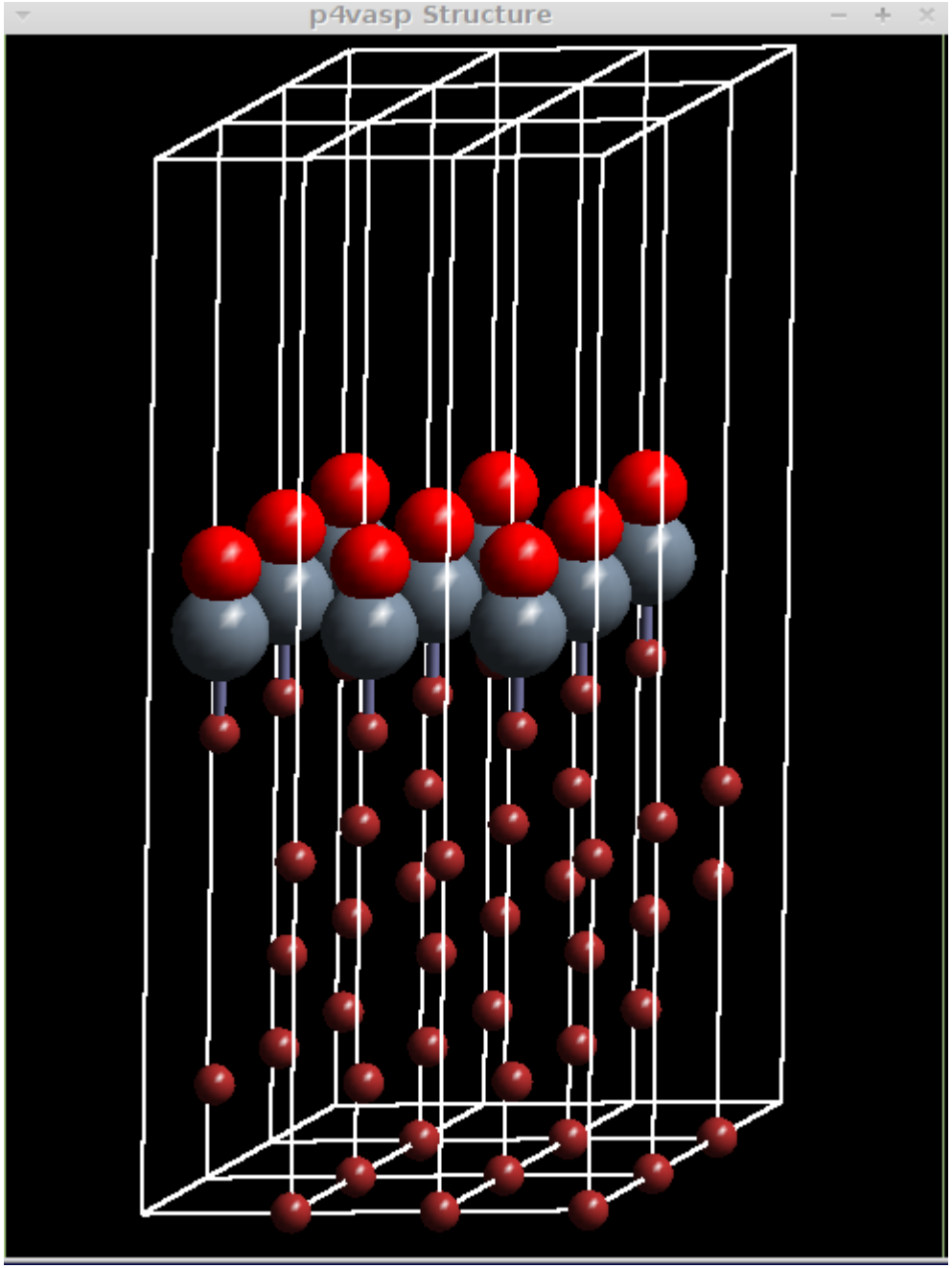
CO@Ni(111) (Example: 3_5_COonNi111_rel)

Geometry:

POSITION			TOTAL-FORCE (eV/Angst)		
0.00000	0.00000	0.00000	0.000000	0.000000	0.175780
0.00000	1.44112	2.03805	0.000000	0.000000	-0.104008
1.24804	0.72056	4.07609	0.000000	0.000000	-0.036305
0.00000	0.00000	6.10852	0.000000	0.000000	-0.083336
0.00000	1.44112	8.15366	0.000000	0.000000	0.009539
0.00000	1.44112	9.90873	0.000000	0.000000	0.011228
0.00000	1.44112	11.06339	0.000000	0.000000	0.027102
total drift:			-0.000093	-0.000213	0.019852

- small outward relaxation of surface due to adsorption
  $\Rightarrow \Delta d_{12} = (8.154 - 6.109)/2.038 = 0.4\%$
- CO geometry
  $\Rightarrow d_{CO} = 11.063 - 9.909 = 1.155\text{Å}; z_C = 9.909 - 8.154 = 1.755\text{Å}.$

CO@Ni(111) (Example: 3_5_COonNi111_rel)



Ni(111) with higher cutoff (Example: 3_6_Ni111clean_400eV)

Run a single point calculation for the Ni(111) clean surface at a higher cutoff (400eV), (needed to compute the adsorption energy)

- potentials for oxygen and carbon require an energy cut-off of 400 eV.
  $\Rightarrow$ previous calculation for clean cannot be used as reference
  $\Rightarrow$ recalculate with same energy cut-off

```
  ENMAX = 400

 general:
   ISTART = 0
   ICHARG = 2
   ISMEAR =    2
   SIGMA = 0.2
   ALGO= Fast

 special:
   LVHAR = .TRUE.
#  LVTOT = .TRUE.
```

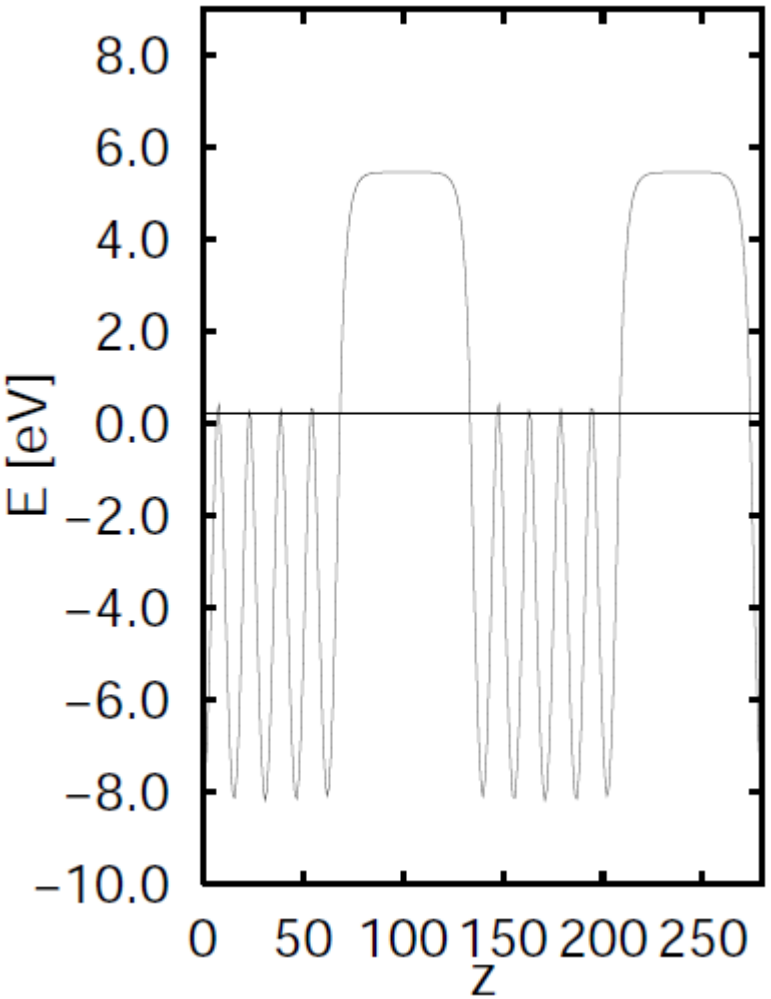
INCAR

- change of cut-off lowers total energy
  $\Rightarrow$ –25.732 eV (270 eV) $\rightarrow$ –25.737 eV at 400 eV
  $\Rightarrow$ becomes more important for larger cells!
- $E_{\text{ads}} = E_{\text{total}} - E_{\text{clean}} - E_{\text{CO}}$
  $\Rightarrow E_{\text{ads}} = -40.829 + 25.737 + 14.835 = -0.257$ eV
- we use this run also to calculate the work-function of Ni(111)

N.B.: the setup for the calculation of the “CO” energy you'll find in the *3_5_COonNi111_rel/CO* subdirectory.

Ni(111) with higher cutoff (Example: 3_6_Ni111clean_400eV)

- use `p4vasp` to show the planar average of the potential
- vacuum-potential $E^{\mathrm{vac}} = 5.45$ eV
- Fermi-level $\varepsilon_{\mathrm{F}} = 0.224$ eV (from OUTCAR)
- $\boxed{\Phi = E^{\mathrm{vac}} - \varepsilon_{\mathrm{F}}} = 5.23$ eV



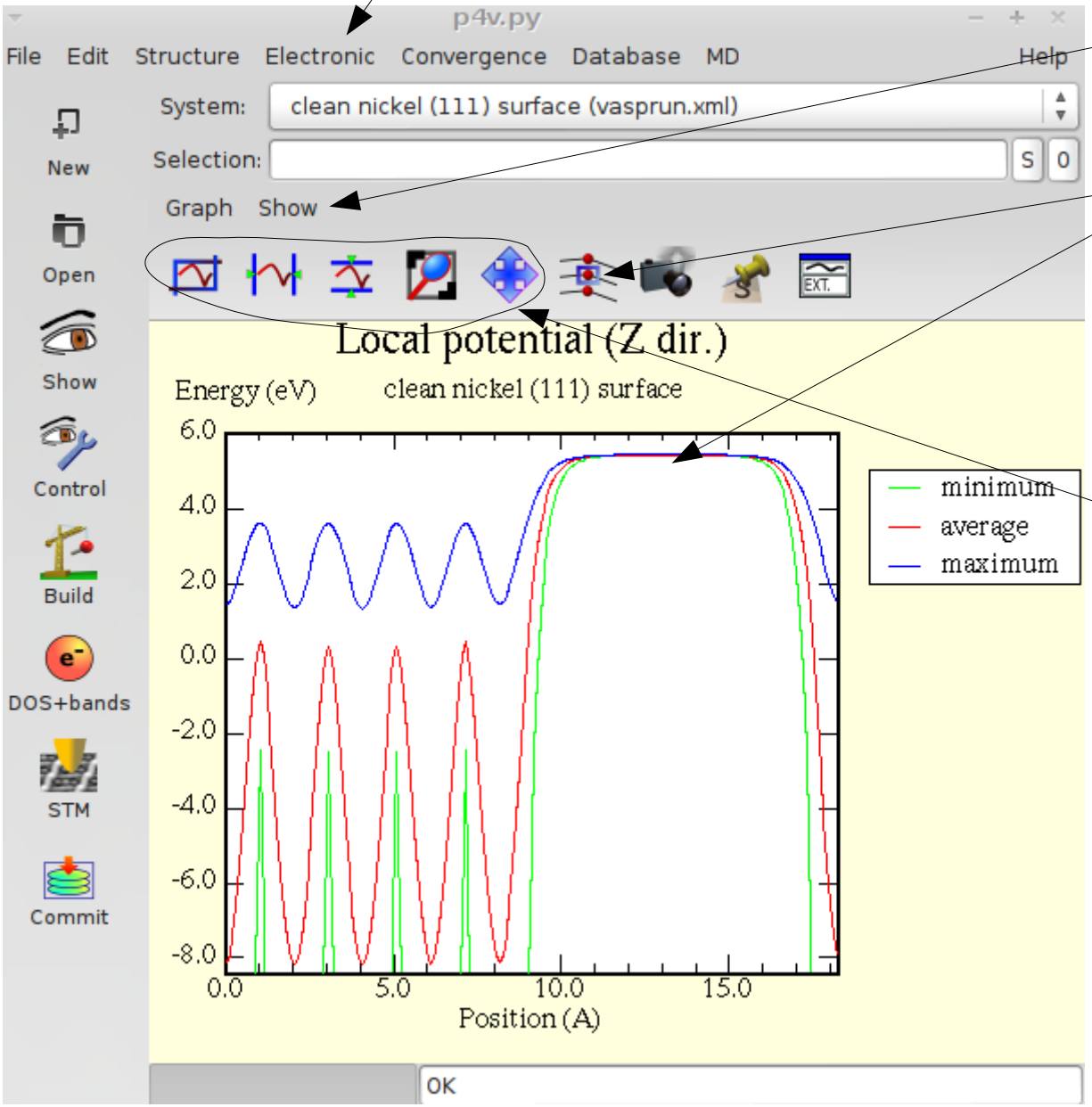
Ni(111) with higher cutoff (Example: 3_6_Ni111clean_400eV)

Go to “Electronic/Local potential”

Select “Z - direction”

“Measure” point in graph

Zoom to area of interest



CO@Ni(111) LDOS&workfunction (Example: 3_7_COonNi111_LDOS)

```
 general:
   ENMAX = 400
   SYSTEM = CO adsorption on Ni(111)
   ISMEAR = -5
   ALGO= Fast

 LDOS:
   LORBIT = 11

 workfunction:
   IDIPOL=3
   LDIPOL= .TRUE.
   LVHAR = .TRUE.
#  LVTOT = .TRUE.
```

INCAR

- for DOS calculation `ISMEAR=-5`
- `LVHAR` writes Hartree part of the local potential to `LOCPOT`
- `LVTOT` writes total local potential into `LOCPOT` file
- `IDIPOL` enables dipole correction in direction 3
- active dipole corrections to potential (=dipole layer)

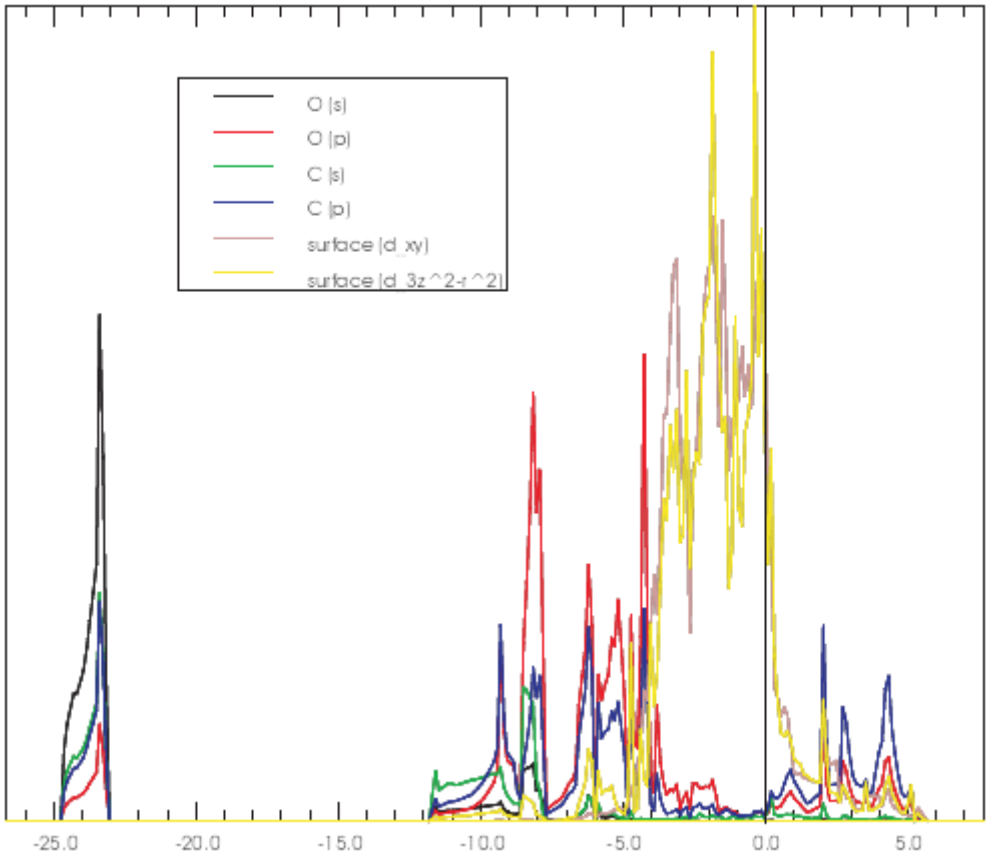
N.B.: We want to use the optimized structure of 3_5_COonNi111_rel:

Normally this would mean copying the CONTCAR of 3_5_COonNi111_rel to POSCAR in the directory where you want to run 3_7_COonNi111_LDOS.

In this case, however, that has already been taken care of, andthe POSCAR file in 3_7_COonNi111_LDOS is already the correct one.

CO@Ni(111) LDOS&workfunction (Example: 3_7_COonNi111_LDOS)

- lm-decomposed DOS helps to analyze the bonding
- CO $5\sigma, 1\pi, 2\pi^*$
- from comparison with substrate LDOS
  - hybridization with Ni-$d_{3z^2-r^2}$
  - no interaction with d_{xy}
    $\Rightarrow$ from symmetry

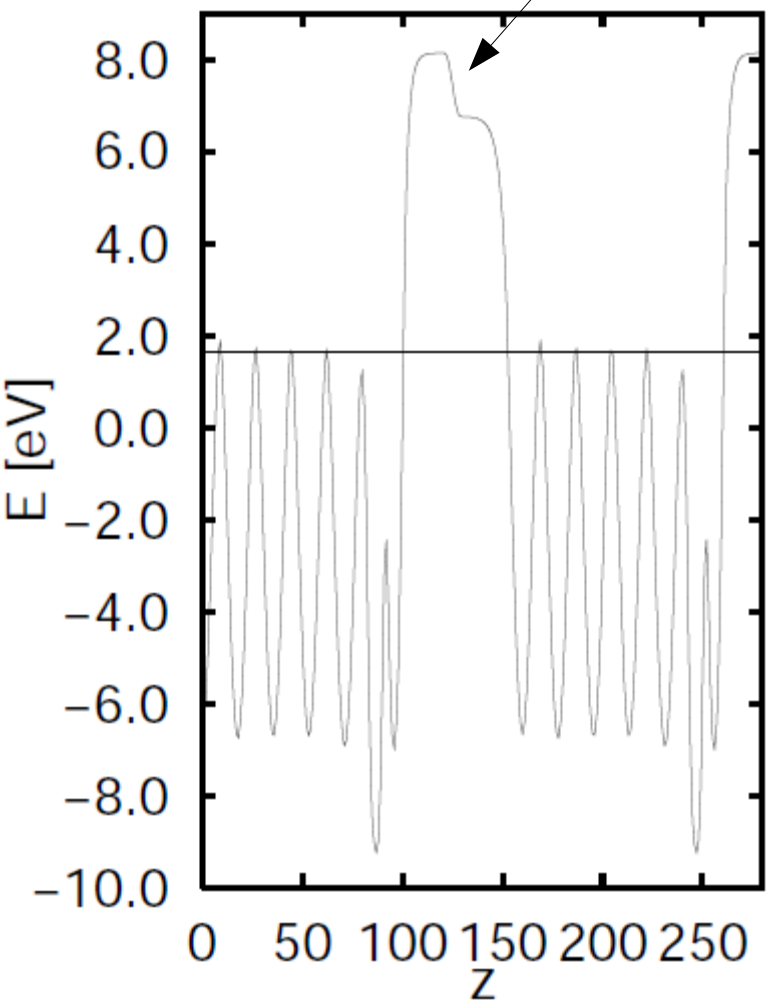


Visualisation: use p4vasp as explained for example 3_2_Ni100clean_LDOS.

CO@Ni(111) LDOS&workfunction (Example: 3_7_COonNi111_LDOS)

- $\varepsilon_F = 1.65$ eV (from OUTCAR)
- vacuum-potential at 8.24 / 6.77 eV
  $\Rightarrow \Phi_{CO} = 6.58, \Phi_{clean} = 5.11$ eV
- too small result for clean surface due to too small vacuum ...

Due to the dipole corrections!



Visualisation: use p4vasp as explained for example 3_6_Ni111clean_400eV.

CO@Ni(111) vibrational frequencies (Example: 3_8_COonNi111_freq)

```
 SYSTEM= CO on Ni111 - frequencies

general:
  ENMAX  = 400
  ISMEAR =    2  ; SIGMA = 0.2
  ALGO   = Fast
  EDIFF  = 1E-6
  MAXMIX = 60

dynamic:
  NSW=100
  IBRION = 5
  NFREE  = 2
```

INCAR

- the very usual settings ...
- smaller termination criterion EDIFF
- automatic frequency calculation (displacement 0.04 Å)
- MAXMIX: reuse the mixer between ionic steps, saves time

CO@Ni(111) vibrational frequencies (Example: 3_8_COonNi111_freq)

```
 Ni - (111) + CO ontop
   3.53000000000000
     0.70710678   0.00000000   0.00000000
    -0.35355339   0.61237240   0.00000000
     0.00000000   0.00000000   5.19615239
   5   1   1
Selective dynamics
Direct
  0.00000000  0.00000000  0.00000000   F   F   F
  0.33333333  0.66666666  0.11111111   F   F   F
  0.66666666  0.33333333  0.22222221   F   F   F
  0.00000000  0.00000000  0.33303912   F   F   F
  0.33333333  0.66666666  0.44454220   F   F   F
  0.33333333  0.66666666  0.54020250   F   F   T
  0.33333333  0.66666666  0.60315365   F   F   T
```

- frequencies only for CO molecule and z-direction (z- and (x,y) are independent!)

N.B.: We want to use the optimized structure of 3_5_COonNi111_rel:

Normally this would mean copying the CONTCAR of 3_5_COonNi111_rel to POSCAR in the directory where you want to run 3_8_COonNi111_freq, and specifying the appropriate degrees-of-freedom.

In this case, however, that has already been taken care of, andthe POSCAR file in 3_8_COonNi111_freq is already the correct one.

CO@Ni(111) vibrational frequencies (Example: 3_8_COonNi111_freq)

Additional output in OUTCAR file for frequency calculation via finite difference:

```
Finite differences progress:
 Degree of freedom:   1/  2
 Displacement:        1/  2
 Total:               1/  4
```

- After the first calculation for the equilibrium geometry, NFREE displacements (± POTIM) are performed for each degree of freedom; from these displacements the dynamical matrix is set up and diagonalized
- at the end of the OUTCAR file the
  - forces,
  - the dynamical matrix and finally
  - the eigenfrequencies and
  - eigenvectors (first normalized and then mass-weighted)

  are listed

CO@Ni(111) vibrational frequencies (Example: 3_8_COonNi111_freq)

```
Eigenvectors and eigenvalues of the dynamical matrix
----------------------------------------------------
  1 f  =   63.914144 THz   401.584411 2PiTHz 2131.946301 cm-1   264.327748 meV
            X         Y         Z           dx          dy          dz
     0.000000  0.000000  0.000000            0           0           0
     0.000000  1.441116  2.038046            0           0           0
     1.248043  0.720558  4.076093            0           0           0
     0.000000  0.000000  6.108743            0           0           0
     0.000000  1.441116  8.153979            0           0           0
     0.000000  1.441116  9.908620            0           0   -0.781748
     0.000000  1.441116 11.063296            0           0    0.623594

  2 f  =   12.467410 THz    78.335050 2PiTHz  415.868035 cm-1    51.561083 meV
            X         Y         Z           dx          dy          dz
     0.000000  0.000000  0.000000            0           0           0
     0.000000  1.441116  2.038046            0           0           0
     1.248043  0.720558  4.076093            0           0           0
     0.000000  0.000000  6.108743            0           0           0
     0.000000  1.441116  8.153979            0           0           0
     0.000000  1.441116  9.908620            0           0   -0.623594
     0.000000  1.441116 11.063296            0           0   -0.781748
```

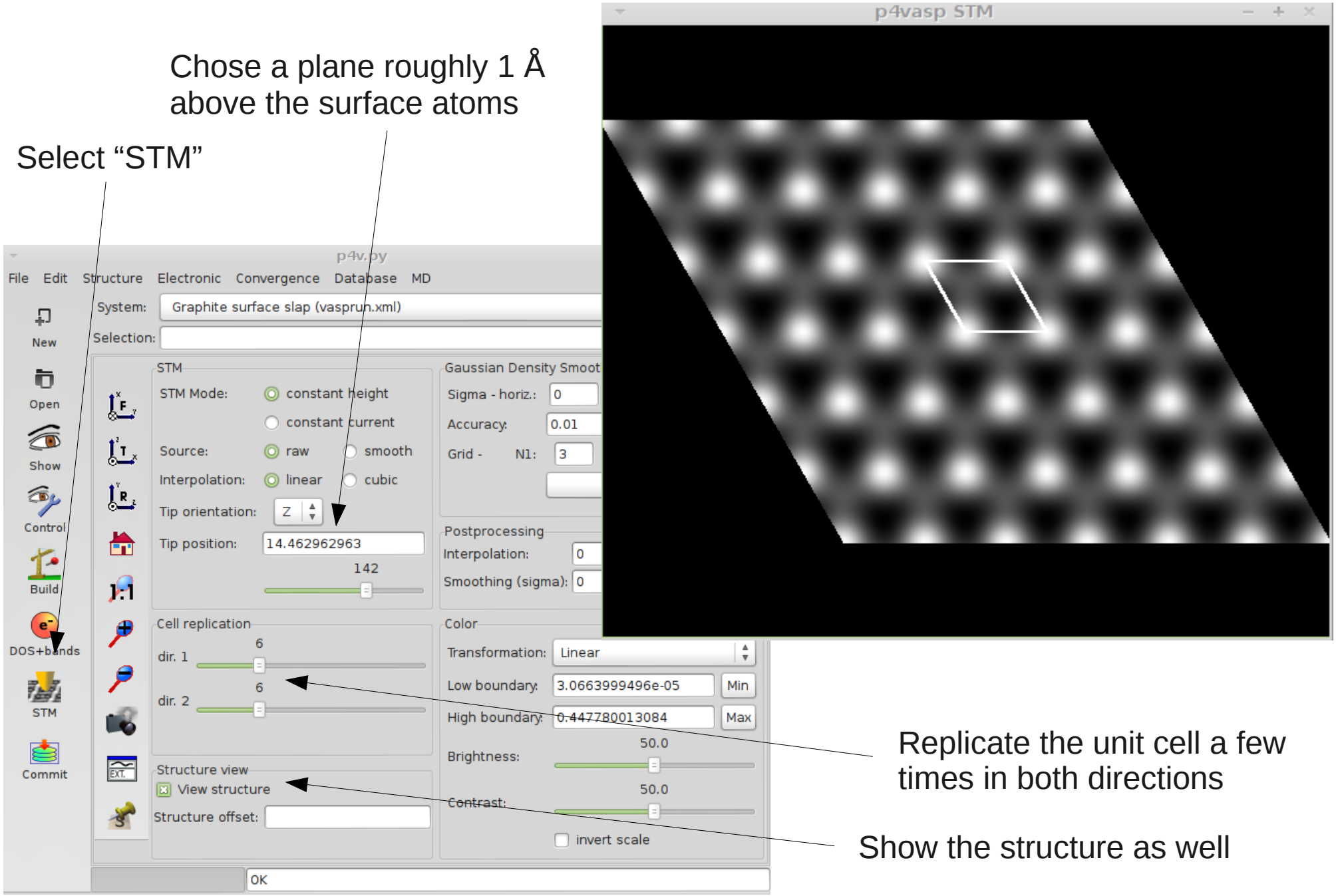
CO stretch

CO-metal

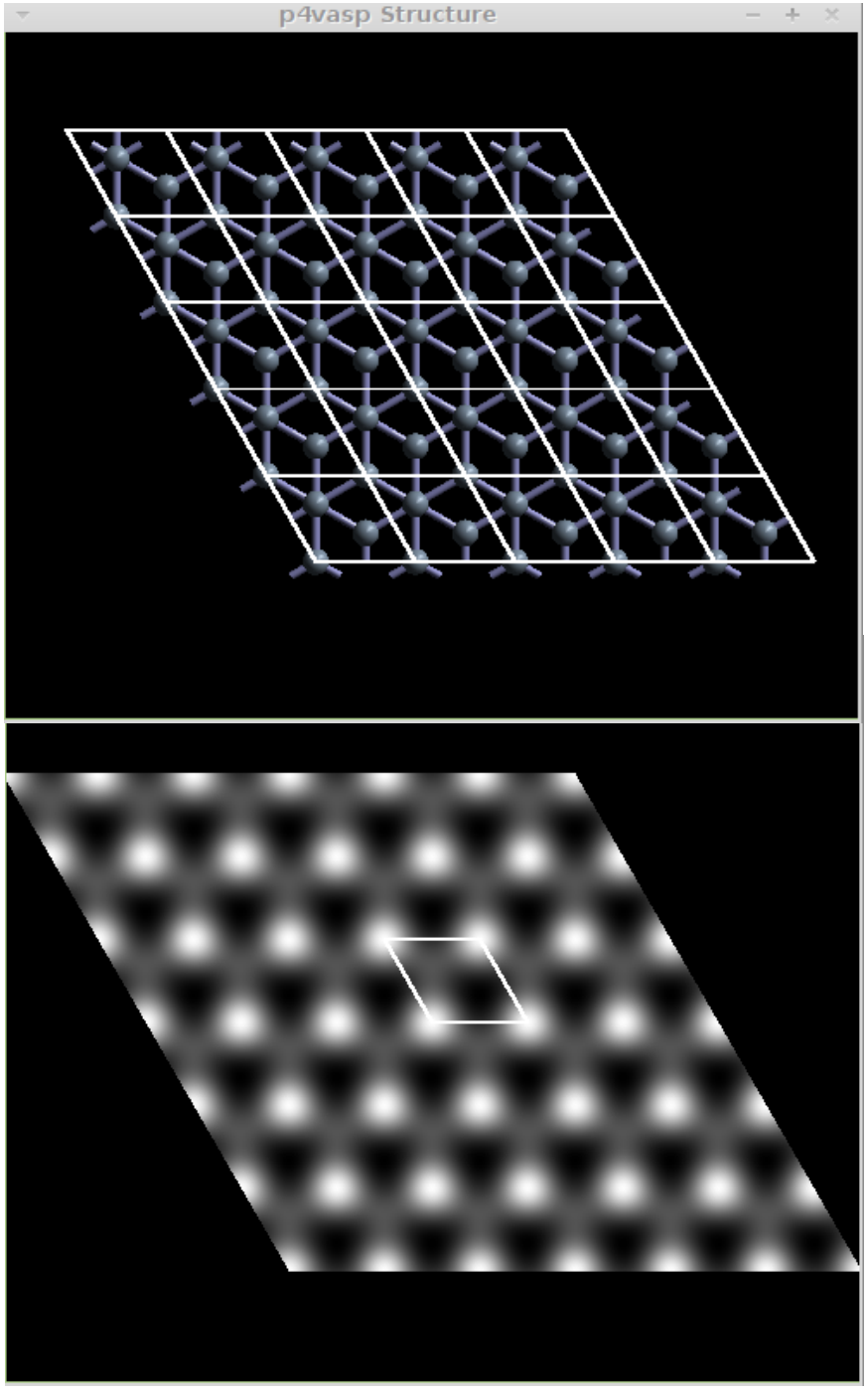
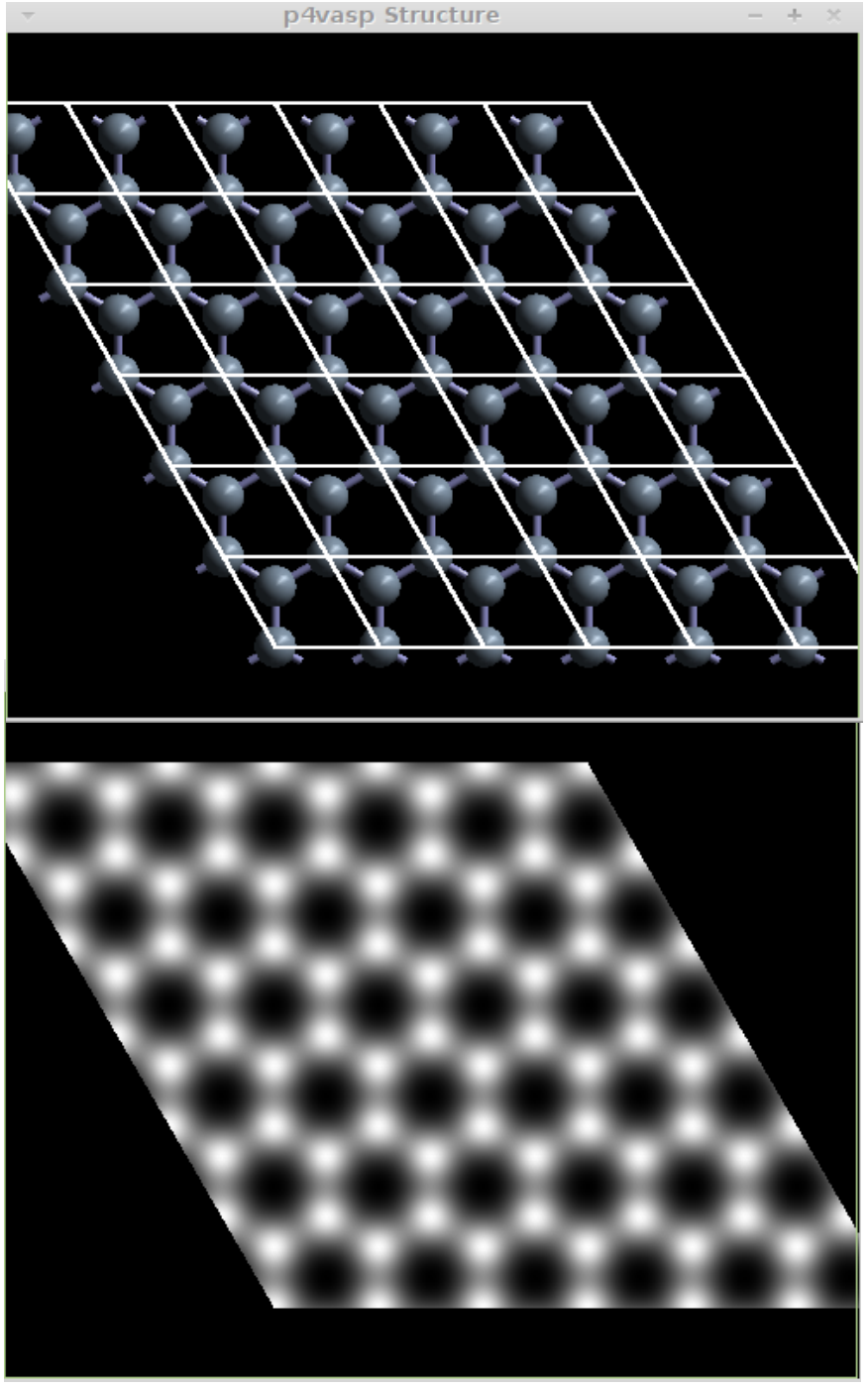
STM (Examples: 3_9_Graphite_STM and 3_10_Graphene_STM)

Chose a plane roughly 1 Å above the surface atoms

Select “STM”



Replicate the unit cell a few times in both directions

Show the structure as well

STM (Examples: 3_9_Graphite_STM and 3_10_Graphene_STM)