VASP Tutorial:
Atoms, molecules, and bulk systems

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Setting up a VASP calculation

VASP requires 4 input files to run a calculation:

- INCAR
- POSCAR
- KPOINTS
- POTCAR

I: The INCAR file

The INCAR file contains the input parameters that steer the calculation:

- The default values set by VASP itself are a clever choice for most standard calculations

- These standard settings may be modified to specify:

    - What kind of calculation you want to do:
      SCF calculation, DOS, dielectric properties, …

    - Basic inputs concering the required precision, the requested level of convergence, ...

For a list of all INCAR-tags have a look at:

- 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

II: The POSCAR file

In the POSCAR file you specify the structure (Bravais lattice and basis):

fcc: Ni	Header (comment)
3.53	Overall scaling constant
0.5 0.5 0.0 0.0 0.5 0.5 0.5 0.0 0.5	Bravais matrix
Ni	Name(s) of atomic type(s)
1	Number of atoms (of each type)
Selective Dynamics	(optional: selective dynamics)
Cartesian	Cartesian or Direct coordinates
0 0 0 (T T T)	positions of the atoms

III: The KPOINTS file

In the KPOINTS file you specify the points VASP will use to sample the first Brillouin zone in reciprocal space

`Automatic mesh`	Header (comment)
`0`	N_k=0: automatic mesh generation
`G (M)`	**Γ**-centered (G) mesh or Monkhorst-Pack (M) grid
`4 4 4`	# of subdivisions N_i along $\vec{b}_i$
`0. 0. 0.`	Optionally shift the mesh (s_i)

IV: The POTCAR file

The POTCAR file has to contain the PAW datasets for all atomic types you have specified in your POSCAR file:

VASP comes with a library of PAW datasets, (one or more) for most elements of the periodic table:

- Each individual PAW data set starts with a descriptive section, specifying amongst other things:
    - Parameters that were required to generate the dataset:
    - Number of valence electrons
    - Atomic mass
    - Default energy cutoffs

- When your unit cell contains more than one type of atom you have to concatenate the corresponding PAW datasets in the same order as you have specified the different atomic types in your POSCAR file.

- You should not mix PAW datasets generated with different exchange-correlation functionals.

OUTPUT files

OUTCAR

- detailed output of a VASP run, including:
  - a summary of the input parameters
  - information about the individual electronic steps: total energy, Kohn-Sham eigenvalues, Fermi-energy.
  - stress tensors
  - forces in the atoms
  - local charges, magnetic moments
  - dielectric properties
  - ... and a great many things more ...
- The amount of output written onto OUTCAR can be chosen by means of the NWRITE-tag in the INCAR file.

OSZICAR & stdout

- give a short summary of the self-consistency-cycle
  - chosen SCF algorithm
  - convergence of energy and charge density
  - free energies, total magnetic moment of the cell

OUTPUT files

CONTCAR & XDATCAR

- CONTCAR: updated geometry data *at the end of a run*
    - lattice parameter
    - Bravais matrix
    - ionic positions
    - velocities
- the format of the CONTCAR is the same as for POSCAR:
  It can be directly be used for a continuation run (copy
  CONTCAR to POSCAR)
- XDATCAR: updated ionic positions of each ionic step

DOSCAR, CHGCAR & WAVECAR

- DOSCAR: total DOS and integrated DOS, (local partial DOS)
- CHGCAR: the charge density
- WAVECAR: plane wave coefficients of the orbitals.
  Can be used to restart from a previous run

Atoms and Molecules

Examples:

- O atom
- O_2 dimer
- CO
- H_2O

Tasks:

- Single point total energy
- Relaxation
- Vibrational frequencies
- MD

The oxygen atom (ex.: O atom)

The POSCAR file specifies the Bravais lattice (lattice vectors) and basis (atomic positions).

- In this case, a single atom in a box:

`O atom in a box`	`Header (comment)`
`1.0`	`Overall scaling constant`

`8.0 0.0 0.0`
`0.0 8.0 0.0`
`0.0 0.0 8.0`
	`lattice vector a(1)`
	`lattice vector a(2)`
	`lattice vector a(3)`

`1`	`Number of atoms`
`cart`	`Positions in cartesian coordinates`
`0 0 0`	`positions of atom 1`

The INCAR file steers the calculation

`SYTEM = O atom in a box`	`Name of the calculation`
`ISMEAR = 0`	`Selects Gaussian smearing`

The oxygen atom (ex.: O atom)

The KPOINTS file determines which Bloch wave vectors $\{\vec{k}\}$ are used to sample the first Brillouin zone.

- For atoms or molecules only a single **k**-point is used: $\vec{k} = 0$ (the **Γ**-point)

- Were more/other **k**-points to be used, only the interaction *between the periodically repeated images of the atom or molecule,* that we'd like to be zero, are described moreaccurately.

The KPOINTS file:

Gamma-point only	Header (comment)
0	N_k=0: automatic mesh generation
Monkhorst-Pack	Monkhorst-Pack grid
1 1 1	# of subdivisions N_i along $\vec{b}_i$
0. 0. 0.	Optionally shift the mesh (s_i)

The oxygen atom (ex.: O atom)

Running VASP should yield the following on *stdout* (and much the same on OSZICAR):

```
 running on    8 total cores
 distrk:  each k-point on    8 cores,    1 groups
 distr:  one band on    1 cores,    8 groups
 using from now: INCAR
 vasp.5.4.1 05Feb16 (build Aug 22 2016 16:46:23) complex

 POSCAR found :  1 types and       1 ions
 scaLAPACK will be used
 LDA part: xc-table for Pade appr. of Perdew
 POSCAR, INCAR and KPOINTS ok, starting setup
 WARNING: small aliasing (wrap around) errors must be expected
 FFT: planning ...
 WAVECAR not read
 entering main loop
       N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1     0.384469664751E+02    0.38447E+02   -0.96726E+02    16   0.293E+02
DAV:   2     0.345965628955E+01   -0.34987E+02   -0.34942E+02    32   0.450E+01
DAV:   3    -0.244485866931E+00   -0.37041E+01   -0.34307E+01    16   0.308E+01
DAV:   4    -0.312557021227E+00   -0.68071E-01   -0.66914E-01    16   0.508E+00
DAV:   5    -0.313520305300E+00   -0.96328E-03   -0.96311E-03    32   0.506E-01    0.286E-01
DAV:   6    -0.314540466589E+00   -0.10202E-02   -0.17853E-03    16   0.332E-01    0.142E-01
DAV:   7    -0.314637222361E+00   -0.96756E-04   -0.22710E-04    16   0.134E-01
   1 F= -.31463722E+00 E0= -.16037490E+00  d E =-.308525E+00
 writing wavefunctions
```

The oxygen atom (ex.: O atom)

```
entering main loop
       N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1     0.384469664751E+02    0.38447E+02   -0.96726E+02    16   0.293E+02
DAV:   2     0.345965628955E+01   -0.34987E+02   -0.34942E+02    32   0.450E+01
DAV:   3    -0.244485866931E+00   -0.37041E+01   -0.34307E+01    16   0.308E+01
DAV:   4    -0.312557021227E+00   -0.68071E-01   -0.66914E-01    16   0.508E+00
DAV:   5    -0.313520305300E+00   -0.96328E-03   -0.96311E-03    32   0.506E-01    0.286E-01
DAV:   6    -0.314540466589E+00   -0.10202E-02   -0.17853E-03    16   0.332E-01    0.142E-01
DAV:   7    -0.314637222361E+00   -0.96756E-04   -0.22710E-04    16   0.134E-01
   1 F= -.31463722E+00 E0= -.16037490E+00  d E =-.308525E+00
 writing wavefunctions
```

OSZICAR and stdout	
N	Iteration count
E	Total energy
dE	Change of total energy
d eps	Change in the eigenvalues (at fixed potential)
ncg	Number of times $H\psi$ is evaluated (essential part of optimization)
rms	Total residual vector $\sum_{nk} w_k f_{nk} (H - \varepsilon_{nk}) \psi_{nk}$
rms(c)	Charge-density residual vector

- The initial charge density corresponds to the charge of overlapping atomic charge densities (from the POTCAR file). For 4 steps the charge density was kept fixed, thereafter it was updated (see the `rms(c)` column).

The oxygen atom (ex.: O atom)

The main output of VASP is written to the OUTCAR file. It contains several section, separated by lines like the following:

```
-----------------------------------------------------------
```

The sections are:

- first part: reading INCAR, POTCAR, POSCAR
- nearest neighbor distances and analysis of symmetry
- information on what was parsed from INCAR
- verbose job information
- information on lattice, k-points and positions
- information on the basis set (number of plane waves)
- non local pseudopotential information
- information for each electronic step (one line in OSZICAR)

The oxygen atom (ex.: O atom)

- Timing and energy information:

```
   POTLOK:  cpu time    0.0878: real time    0.0877
   SETDIJ:  cpu time    0.0015: real time    0.0014
    EDDAV:  cpu time    0.0267: real time    0.0434
      DOS:  cpu time    0.0001: real time    0.0001
   --------------------------------------------
     LOOP:  cpu time    0.1165: real time    0.1346

eigenvalue-minimisations  :    16
total energy-change (2. order) : 0.3844697E+02  (-0.9672571E+02)
number of electron       6.0000000 magnetization
augmentation part        6.0000000 magnetization

Free energy of the ion-electron system (eV)
 ---------------------------------------------------
 alpha Z        PSCENC =         0.27135287
 Ewald energy   TEWEN  =       -91.92708002
 -Hartree energ DENC   =      -281.84385691
 -exchange      EXHF   =         0.00000000
 -V(xc)+E(xc)   XCENC  =        26.11948841
 PAW double counting   =       245.99840262     -247.84808825
 entropy T*S    EENTRO =        -0.08636665
 eigenvalues    EBANDS =       -44.50008162
 atomic energy  EATOM  =       432.26319604
 Solvation  Ediel_sol  =         0.00000000
 ---------------------------------------------------
 free energy    TOTEN  =        38.44696648 eV

 energy without entropy =       38.53333313  energy(sigma->0) =       38.49014980
```

The oxygen atom (ex.: O atom)

- Eigenvalues:

```
E-fermi :  -8.8431     XC(G=0):  -0.8043     alpha+bet : -0.1463


 k-point     1 :       0.0000    0.0000    0.0000
  band No.  band energies     occupation
      1     -23.8439      2.00000
      2      -8.9040      1.33333
      3      -8.9040      1.33333
      4      -8.9040      1.33333
      5      -0.4676      0.00000
      6       1.8633      0.00000
      7       1.8633      0.00000
      8       1.8633      0.00000
```

The oxygen atom (ex.: O atom)

- Information on stress tensor:

```
FORCE on cell =-STRESS in cart. coord.  units (eV):
 Direction    XX          YY          ZZ          XY          YZ          ZX
 --------------------------------------------------------------------------------------
 Alpha Z     0.27135     0.27135     0.27135
 Ewald     -30.64236   -30.64236   -30.64236     0.00000     0.00000     0.00000
 Hartree    93.90244    93.90244    93.90244    -0.00000    -0.00000    -0.00000
 E(xc)     -27.93035   -27.93035   -27.93035    -0.00000    -0.00000    -0.00000
 Local    -147.86211  -147.86211  -147.86211     0.00000     0.00000     0.00000
 n-local   -20.54942   -20.54942   -20.54942    -0.00000    -0.00000    -0.00000
 augment     5.55366     5.55366     5.55366     0.00000    -0.00000     0.00000
 Kinetic   126.50998   126.50998   126.50997    -0.00000     0.00000    -0.00000
 Fock        0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
 -------------------------------------------------------------------------------------
 Total      -0.74681    -0.74681    -0.74681     0.00000    -0.00000    -0.00000
 in kB      -2.33695    -2.33695    -2.33695     0.00000    -0.00000    -0.00000
 external pressure =       -2.34 kB  Pullay stress =        0.00 kB
```

- and energy:

```
FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)
 ---------------------------------------------------
 free  energy   TOTEN  =        -0.31463722 eV

 energy  without entropy=       -0.00611258  energy(sigma->0) =       -0.16037490
```

The oxygen atom (ex.: O atom)

- the relevant energy for atoms and molecules is energy without entropy:

  ```
  energy  without entropy=       -0.00611258  energy(sigma->0) =       -0.16037490
  ```

  three degenerate p orbitals occupied by 2/3 electrons causing a unphysical electronic entropy

  ```
  entropy T*S    EENTRO =        -0.30852464
  ```

- a tiny value for `SIGMA=0.01` would reduce the entropy but might slow convergence (default is `SIGMA=0.2`).
  `SIGMA` controls the electronic temperature, which is not a very meaningful quantity for atoms and molecules.

- the total energy is found to be essentially zero:
  VASP subtracts from any calculated energy the energy of the atom in the configuration for which the PAW dataset was generated.
  All PAW datasets are generated using non-spinpolarized reference atoms.

The oxygen atom (ex.: O atom)

```
 running on    8 total cores
 distrk:  each k-point on    8 cores,    1 groups
 distr:  one band on    1 cores,    8 groups
 using from now: INCAR
 vasp.5.4.1 05Feb16 (build Aug 22 2016 16:46:23) complex

 POSCAR found :  1 types and       1 ions
 scaLAPACK will be used
 LDA part: xc-table for Pade appr. of Perdew
 found WAVECAR, reading the header
 POSCAR, INCAR and KPOINTS ok, starting setup
 WARNING: small aliasing (wrap around) errors must be expected
 FFT: planning ...
 reading WAVECAR
 the WAVECAR file was read successfully
 initial charge from wavefunction
 entering main loop
       N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1    -0.314680766875E+00   -0.31468E+00   -0.83090E-05    16   0.564E-02    0.107E-02
DAV:   2    -0.314677281013E+00    0.34859E-05   -0.10030E-05    16   0.198E-02
   1 F= -.31467728E+00 E0= -.16041496E+00  d E =-.308525E+00
 writing wavefunctions
```

- When VASP is restarted the WAVECAR file is read and the run continues from the previous wavefunctions (converging rapidly).

The O atom (ex.: O atomspin)

- The O atom is an open-shell system with 2 unpaired electrons.
- add `ISPIN=2` to the INCAR file, remove the WAVECAR file, and restart VASP:

```
 running on    8 total cores
 distrk:  each k-point on    8 cores,    1 groups
 distr:  one band on    1 cores,    8 groups
 using from now: INCAR
 vasp.5.4.1 05Feb16 (build Aug 22 2016 16:46:23) complex

 POSCAR found :  1 types and       1 ions
 scaLAPACK will be used
 LDA part: xc-table for Pade appr. of Perdew
 POSCAR, INCAR and KPOINTS ok, starting setup
 WARNING: small aliasing (wrap around) errors must be expected
 FFT: planning ...
 WAVECAR not read
 entering main loop
       N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1     0.389725012498E+02    0.38973E+02   -0.10098E+03    32   0.259E+02
DAV:   2     0.317912429240E+01   -0.35793E+02   -0.35786E+02    64   0.438E+01
DAV:   3    -0.119085682530E+01   -0.43700E+01   -0.36686E+01    32   0.328E+01
DAV:   4    -0.126198272139E+01   -0.71126E-01   -0.69189E-01    32   0.508E+00
DAV:   5    -0.126284205021E+01   -0.85933E-03   -0.85925E-03    48   0.504E-01     0.653E+00
DAV:   6     0.164008071667E+00    0.14269E+01   -0.32208E+00    32   0.894E+00     0.151E+00
…    …      …
DAV:  13    -0.167302579657E+01   -0.25698E-03   -0.13177E-05    32   0.203E-02     0.956E-03
DAV:  14    -0.167302926747E+01   -0.34709E-05   -0.34771E-06    32   0.116E-02
   1 F= -.16730293E+01 E0= -.15958981E+01  d E =-.154262E+00  mag=     1.9999
 writing wavefunctions
```

The spinpolarized O atom (ex.: O atomspin)

```
E-fermi :  -7.1152     XC(G=0):  -0.7730     alpha+bet : -0.1463


spin component 1

k-point     1 :       0.0000    0.0000    0.0000
 band No.  band energies     occupation
      1     -25.0878      1.00000
      2     -10.0830      1.00000
      3     -10.0830      1.00000
      4     -10.0830      1.00000
      5      -0.4932      0.00000
      6       1.8213      0.00000
      7       1.8303      0.00000
      8       1.8303      0.00000

spin component 2

k-point     1 :       0.0000    0.0000    0.0000
 band No.  band energies     occupation
      1     -21.8396      1.00000
      2      -7.0543      0.33333
      3      -7.0543      0.33333
      4      -7.0543      0.33333
      5      -0.3594      0.00000
      6       1.9830      0.00000
      7       1.9830      0.00000
      8       1.9830      0.00000
```

- Eigenstates for spin-up and spin-down are calculated ”separately”.
- In the OUTCAR file one can see two spin components
- Spincomponent “1” has 2 more electrons, corresponding to a magnetization of 2 μ_B

The O atom (ex.: O atomspinlowsym)

- In the GGA most atoms are characterized by a symmetry broken solution. VASP, however, symmetrizes the charge density according to the determined symmetry of the cell.
  Check the OUTCAR file to see what symmetry VASP is using.
- To lower the symmetry simply change the lattice parameters to 7.0, 7.5, and 8.0 in the POSCAR file :

O atom in a box	Header (comment)
1.0	Overall scaling constant
7.0 0.0 0.0 0.0 7.5 0.0 0.0 0.0 8.0	lattice vector a(1) lattice vector a(2) lattice vector a(3)
1	Number of atoms
cart	Positions in cartesian coordinates
0 0 0	positions of atom 1

- reduce SIGMA to SIGMA=0.01 (in the INCAR file).
- Rerun VASP, and you will find a much lower energy:

```
 vasp.5.4.1 05Feb16 (build Aug 22 2016 16:46:23) complex
…     …     …
DAV:  15    -0.189071145737E+01   -0.29321E-03   -0.39183E-05   48   0.478E-02    0.995E-03
DAV:  16    -0.189098921147E+01   -0.27775E-03   -0.39294E-05   40   0.290E-02    0.541E-03
DAV:  17    -0.189104076616E+01   -0.51555E-04   -0.34087E-06   48   0.132E-02
   1 F= -.18910408E+01 E0= -.18910408E+01  d E =-.309633E-20  mag=     1.9998
```

The O_2 dimer (ex.: O dimer)

- POSCAR:

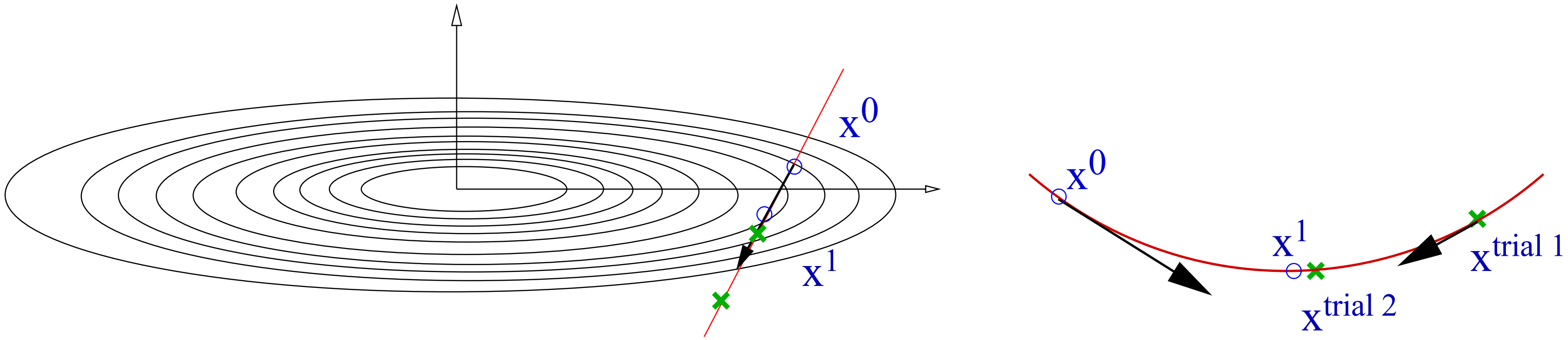
O atom in a box	Header (comment)
1.0	Overall scaling constant
7.0 0.0 0.0 0.0 7.5 0.0 0.0 0.0 8.0	lattice vector a(1) lattice vector a(2) lattice vector a(3)
2	Number of atoms
cart	Positions in cartesian coordinates
0 0 0 0 0 1.22	first atom second atom

- INCAR: structural relaxation of the O_2 dimer

SYTEM = O2 dimer in a box	
ISMEAR = 0	Gaussian smearing
ISPIN = 2	spin-polarized calculation
NSW = 5	5 ionic steps
IBRION = 2	use conjugate gradient algorithm

The O_2 dimer (ex.: O dimer)

- We have specified that the geometry should be relaxed: in this case5 ionic steps (NSW=5) are to be done at most.
  For the relaxation a conjugate gradient algorithm is used (IBRION=2).
- CG requires a line minimization along the search direction:



this is done using a variant of Brent's algorithm:

- Trial step along search direction (gradient scaled by POTIM).
- Quadratic or cubic interpolation using energies and forces at $\vec{x}_0$ and $\vec{x}_1$ allows to determine the approximate minimum.
- Continue minimization if app. minimum is not accurate enough.

The O_2 dimer (ex.: O dimer)

```
DAV:   1     0.517118590134E+02    0.51712E+02   -0.31393E+03    80   0.366E+02
…     …      …
…     …      …
DAV:  14    -0.985349953776E+01   -0.15177E-03   -0.57546E-06    64   0.125E-02    0.371E-03
DAV:  15    -0.985357023804E+01   -0.70700E-04   -0.22439E-06    64   0.741E-03
   1 F= -.98535702E+01 E0= -.98535702E+01  d E =-.985357E+01  mag=     2.0000
 curvature:   0.00 expect dE= 0.000E+00 dE for cont linesearch  0.000E+00
 trial: gam= 0.00000 g(F)=  0.113E+00 g(S)=  0.000E+00 ort = 0.000E+00 (trialstep = 0.100E+01)
 search vector abs. value=  0.113E+00
 bond charge predicted
…     …      …
…     …      …
   2 F= -.96234585E+01 E0= -.96234585E+01  d E =0.230112E+00  mag=     2.0000
 trial-energy change:    0.230112  1 .order    0.190722   -0.113406    0.494850
 step:   0.1397(harm=  0.1864)  dis= 0.00731  next Energy=    -9.861386 (dE=-0.782E-02)
 bond charge predicted
…     …      …
…     …      …
   3 F= -.98607735E+01 E0= -.98607735E+01  d E =-.720327E-02  mag=     2.0000
 curvature:  -0.09 expect dE=-0.900E-05 dE for cont linesearch -0.900E-05
 trial: gam= 0.00000 g(F)=  0.969E-04 g(S)=  0.000E+00 ort =-0.331E-02 (trialstep = 0.828E+00)
 search vector abs. value=  0.969E-04
 reached required accuracy - stopping structural energy minimisation
```

The O_2 dimer (ex.: O dimer)

- The quantity `trial-energy change` is the change of the energy in the trial step
- The first value after `1.order` is the expected energy change calculated from the forces:

  $$\frac{F(\text{start})+F(\text{trial})}{2} \times \text{change of positions}$$

  central difference: the second and third values correspond to:
  $F(\text{start}) \times \text{change of positions}$ and $F(\text{trial}) \times \text{change of positions}$
- The value `step:` is the estimated size of the step leading to a line minimization along the current search direction.
  `harm` is the optimal step using a second order (or harmonic) interpolation.
- The trial step size is controlled by the parameter `POTIM`. The value of `step` times `POTIM` is usually optimal.
- The final positions after the optimisation are stored in CONTCAR.
  You can copy CONTCAR to POSCAR and continue the relaxation.

The CO molecule (ex.: CO)

- POSCAR:

`CO molecule in a box`	Header (comment)
`1.0`	Overall scaling constant

`8.0 0.0 0.0`
`0.0 8.0 0.0`
`0.0 0.0 8.0`
	lattice vector a(1)
	lattice vector a(2)
	lattice vector a(3)

`1 1`	Number of atoms for each species
`cart`	Positions in cartesian coordinates
`0 0 0` `0 0 1.12`	first atom second atom

- POTCAR: is created by the concatenation of two individual POTCAR files, corresponding to O and C, *e.g.*:

```
cat  …/O/POTCAR  .../C/POTCAR  >  POTCAR
```

- A similar relaxation as in the previous case (O_2 dimer) is performed.
  But in this case more steps are required, since the first estimate for the minimum is not very accurate.
  The trial steps are much too long (`POTIM` parameter).

The CO molecule (ex.: CO)

```
 1 F= -.14764064E+02 E0= -.14764064E+02  d E =-.147641E+02
 curvature:   0.00 expect dE= 0.000E+00 dE for cont linesearch  0.000E+00
 trial: gam= 0.00000 g(F)=  0.820E+00 g(S)=  0.000E+00 ort = 0.000E+00 (trialstep = 0.100E+01)
 search vector abs. value=  0.820E+00
 bond charge predicted
…           …        …
…           …        …
…           …        …
   2 F= -.12660858E+02 E0= -.12660858E+02  d E =0.210321E+01
 trial-energy change:    2.103205  1 .order    1.311207   -0.819873    3.442288
 step:   0.1924(harm=  0.1924)  dis= 0.02705  next Energy=   -14.842919 (dE=-0.789E-01)
 bond charge predicted
…           …        …
…           …        …
…           …        …
   3 F= -.14747869E+02 E0= -.14747869E+02  d E =0.161943E-01
 curvature:  -0.10 expect dE=-0.902E-01 dE for cont linesearch -0.902E-01
 ZBRENT: interpolating
 opt :   0.0929  next Energy=   -14.802162 (dE=-0.381E-01)
 bond charge predicted
…           …        …
…           …        …
…           …        …
   4 F= -.14796822E+02 E0= -.14796822E+02  d E =-.327586E-01
 curvature:  -0.04 expect dE=-0.330E-03 dE for cont linesearch -0.330E-03
 trial: gam= 0.00000 g(F)=  0.814E-02 g(S)=  0.000E+00 ort =-0.817E-01 (trialstep = 0.819E+00)
 search vector abs. value=  0.814E-02
 reached required accuracy - stopping structural energy minimisation
```

Vibrational frequencies of CO (ex.: CO vibration)

- INCAR:

`SYTEM = CO molecule in a box`	
`ISMEAR = 0`	Gaussian smearing
`IBRION = 5`	Vibrational spectrum
`NFREE = 2`	Use central differences
`POTIM = 0.02`	0.02 step width
`NSW = 1`	ionic steps must be > 1, that's all

- POSCAR:

`CO molecule in a box`	Header (comment)
`1.0`	Overall scaling constant
`8.0 0.0 0.0`	lattice vector a(1)
`0.0 8.0 0.0`	lattice vector a(2)
`0.0 0.0 8.0`	lattice vector a(3)
`1 1`	Number of atoms for each species
`sel`	Selective dynamics
`cart`	Positions in cartesian coordinates
`0 0 0         F  F  T`	first atom
`0 0 1.143     F  F  T`	second atom

The selected degrees of freedom are displaced, once in the $+\hat{z}$ and once in the $-\hat{z}$ direction, by 0.02 Å. In the present case this means 4 displacements, plus the unperturbed geometry (*i.e.*, a total of five ionic configurations).

Vibrational frequencies of CO (ex.: CO vibration)

- At the end of the OUTCAR file:

```
SECOND DERIVATIVES (NOT SYMMETRIZED)
------------------------------------
              1Z          2Z
 1Z   -114.737304  114.737304
 2Z    114.458316 -114.458316


Eigenvectors and eigenvalues of the dynamical matrix
----------------------------------------------------


  1 f  =   63.887522 THz   401.417139 2PiTHz 2131.058277 cm-1   264.217647 meV
             X         Y         Z           dx          dy          dz
     0.000000  0.000000  0.000000            0           0    -0.655280
     0.000000  0.000000  1.143000            0           0     0.755386

  2 f/i=    0.038494 THz     0.241864 2PiTHz    1.284016 cm-1     0.159198 meV
             X         Y         Z           dx          dy          dz
     0.000000  0.000000  0.000000            0           0    -0.755386
     0.000000  0.000000  1.143000            0           0    -0.655280
```

Eigenstates of CO (ex.: CO states)

- The PROCAR file gives valuable information on the character of the one-electron states:

`LORBIT = 10`	`DOSCAR and` *`l`*`-decomposed PROCAR file`
`LORBIT = 11`	`DOSCAR and lm-decomposed PROCAR file`

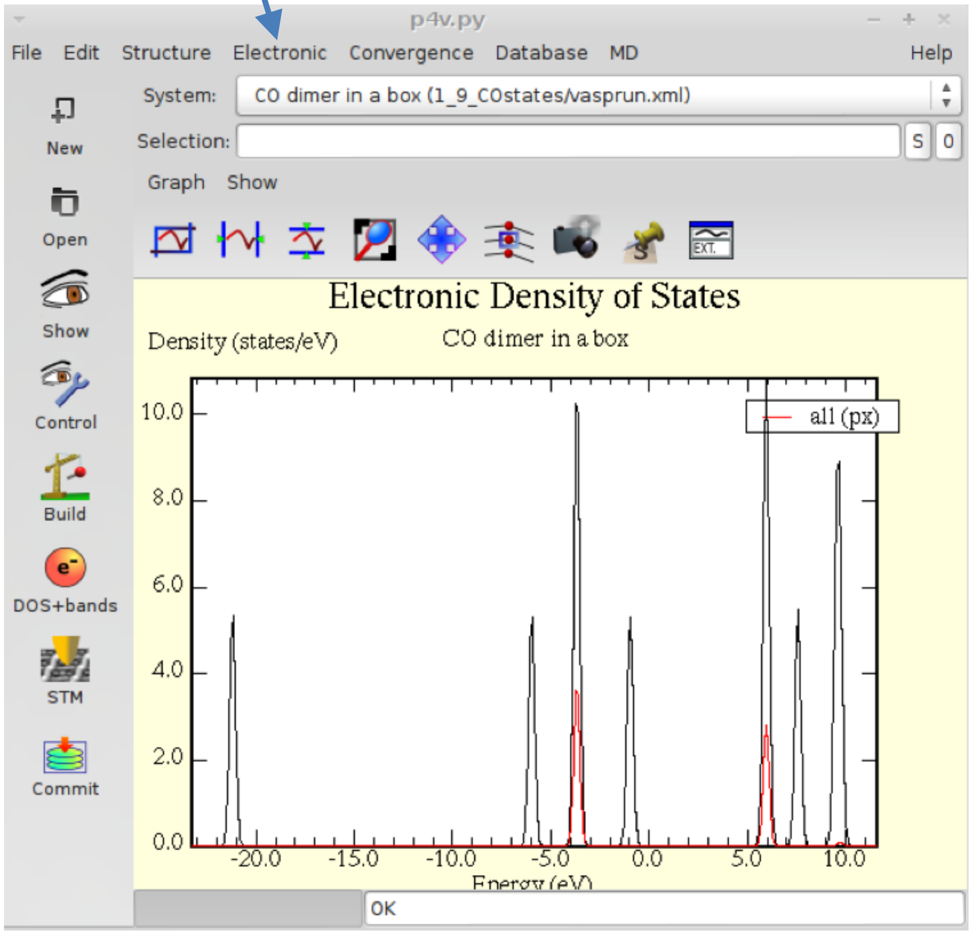
- We'll use LORBIT = 11, and see if we can distinguish p_x and p_y states. Look in the PROCAR file:

```
band   3 # energy  -11.46540832 # occ.  2.00000000

ion      s     py     pz     px    dxy    dyz    dz2    dxz    dx2    tot
  1  0.000  0.510  0.000  0.036  0.000  0.000  0.000  0.000  0.000  0.546
  2  0.000  0.146  0.000  0.010  0.000  0.000  0.000  0.000  0.000  0.157
tot  0.000  0.656  0.000  0.047  0.000  0.000  0.000  0.000  0.000  0.703

band   4 # energy  -11.46540832 # occ.  2.00000000

ion      s     py     pz     px    dxy    dyz    dz2    dxz    dx2    tot
  1  0.000  0.036  0.000  0.510  0.000  0.000  0.000  0.000  0.000  0.546
  2  0.000  0.010  0.000  0.146  0.000  0.000  0.000  0.000  0.000  0.157
tot  0.000  0.047  0.000  0.656  0.000  0.000  0.000  0.000  0.000  0.703

band   5 # energy   -8.76483386 # occ.  2.00000000

ion      s     py     pz     px    dxy    dyz    dz2    dxz    dx2    tot
  1  0.001  0.000  0.135  0.000  0.000  0.000  0.000  0.000  0.000  0.136
  2  0.172  0.000  0.261  0.000  0.000  0.000  0.000  0.000  0.000  0.433
tot  0.173  0.000  0.396  0.000  0.000  0.000  0.000  0.000  0.000  0.569
```

Start p4vasp:

```
> p4v [vasprun.xml]
```

Step 1.) go to:
Electronic/Local DOS+bands control

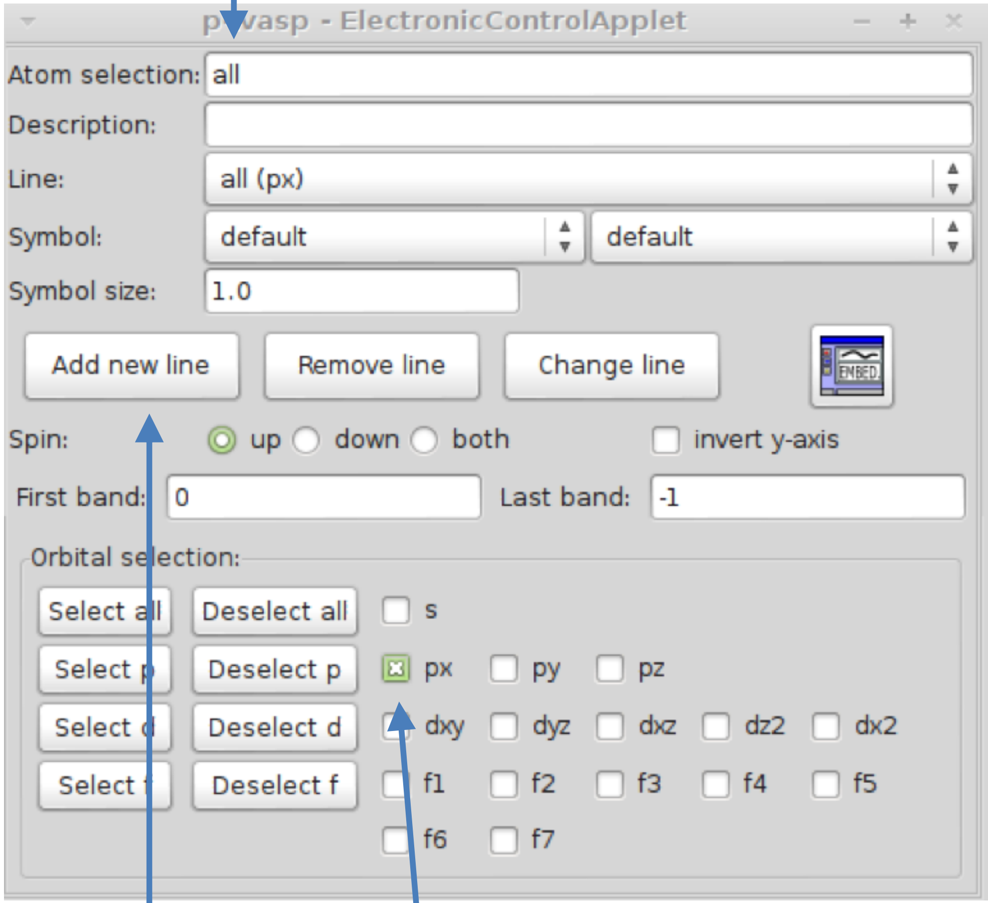


System: CO dimer in a box (1_9_COstates/vasprun.xml)

Selection:

OK

Step 2.) select atoms: “all”, “C”, ”O”, “1”, “2”, …



Atom selection: all

Description:

Line: all (px)

Symbol: default default

Symbol size: 1.0

Spin: ● up ○ down ○ both ☐ invert y-axis

First band: 0 Last band: -1

☐ s
☒ px ☐ py ☐ pz
☐ dxy ☐ dyz ☐ dxz ☐ dz2 ☐ dx2
☐ f1 ☐ f2 ☐ f3 ☐ f4 ☐ f5
☐ f6 ☐ f7

Step 3.) select orbital character

Step 4.) and “Add new line”

The H_2O molecule (ex.: H2O)

- POSCAR:

H2O molecule	Header (comment)
0.52918	Overall scaling constant
15.0 0.0 0.0 0.0 15.0 0.0 0.0 0.0 15.0	lattice vector a(1) lattice vector a(2) lattice vector a(3)
1 2	Number of atoms per species
select	
cart	Positions in cartesian coordinates
0.00 0.00 0.00 F F F 1.10 -1.43 0.00 T T F 1.10 1.43 0.00 T T F	

all coordinates are scaled by the factor 0.52918

- INCAR: structural relaxation of the O_2 dimer

PREC = Normal	Standard precision
ENMAX = 400	Cutoff should be set manually
ISMEAR = 0 ; SIGMA = 0.1	
IBRION = 1	Use DIIS algorithm to relax structure
NFREE = 2	2 independent degrees of freedom
NSW = 10	10 ionic steps
EDIFFG = -0.02	Forces smaller 0.02 Angstroem/eV

The H_2O molecule (relaxation: H2O, vibrations: H2Ovib)

- Use `PREC = Normal` (Default for VASP.5.X)

- It is strongly recommended to set the energy cutoff manually in the INCAR file, as it gives you more control over the calculations and forces you to think about this aspect.

- For the ionic optimisation the DIIS algorithm is used.
  This algorithm builds an approximation of the Hessian matrix and usually converges faster than the conjugate gradient algorithm.
  It is, however, recommended to specify the number of independent degrees-of-freedom manually.

  `EDIFFG` determines when to terminate the ionic relaxation:
  `EDIFFG` > 0: energy change between steps must be less than `EDIFFG`.
  `EDIFFG` < 0: $\left|\vec{F}_i\right| < |\mathrm{EDIFFG}| \quad \forall\, i = 1, \ldots, N_{\mathrm{ions}}$.

MD with the H_2O molecule (ex.: H2Omd)

- INCAR:

`PREC = Normal`	Standard precision
`ENMAX = 400`	Cutoff should be set manually
`ISMEAR = 0 ; SIGMA = 0.1`	
`ISYM = 0`	Strongly recommended for MD
`IBRION = 0`	Molecular Dynamics
`NSW = 1000`	1000 MD steps
`POTIM = 0.5`	Timestep 0.5 fs
`SMASS = -3`	Nose-Hoover thermostat
`TEBEG = 2000 ; TEEND = 2000`	Temperature (begin, end)
`NBANDS = 8`	

time step for this system should be around 0.5-0.7 fs

- POSCAR: to save time the box size is reduced to 12 a.u.

- OSZICAR:

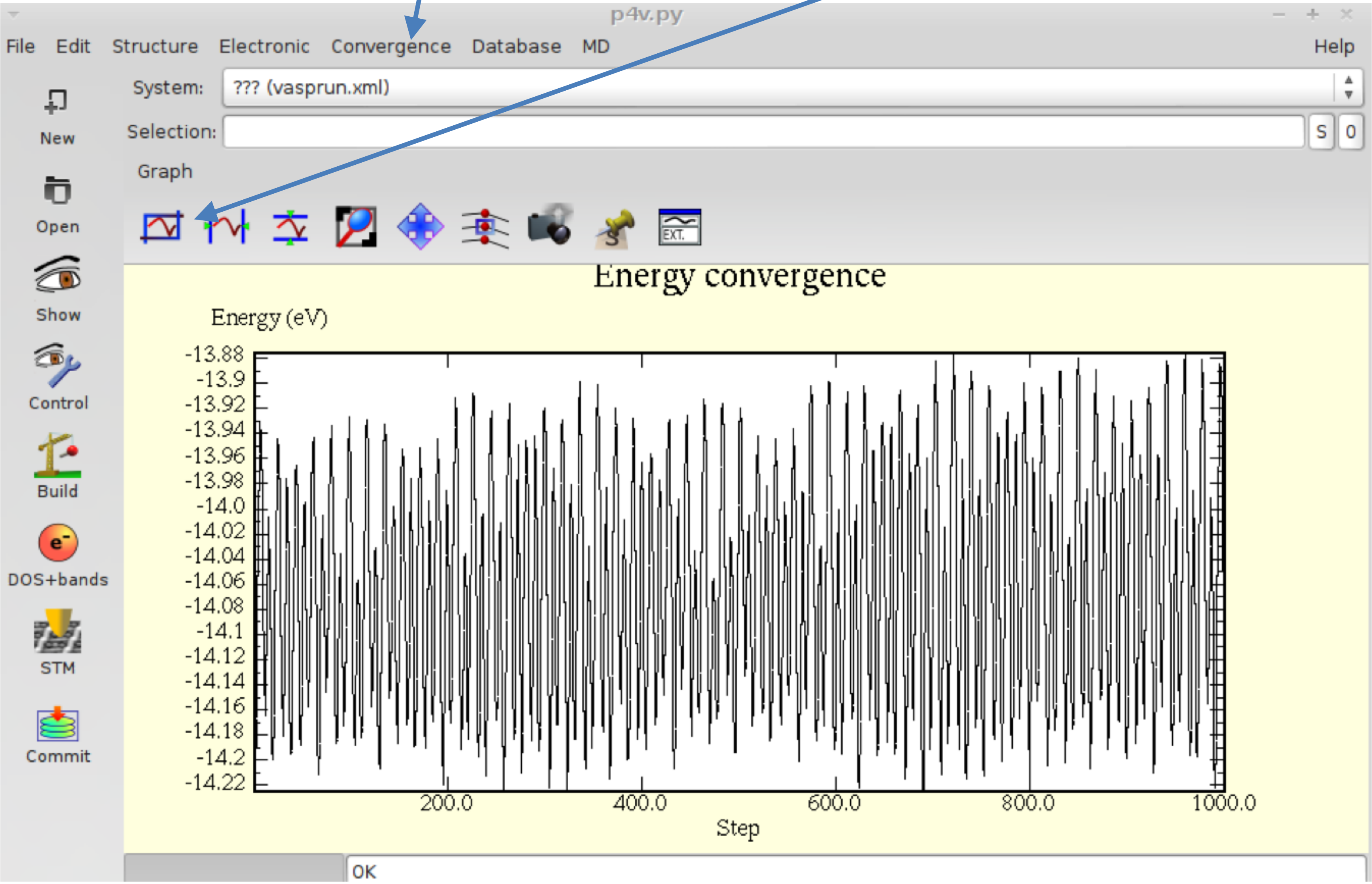
```
1 T=  2134. E= -.13655511E+02 F= -.14207209E+02 E0=.. EK= 0.55170E+00 SP= 0.00E+00 SK= 0.00E+00
2 T=  1971. E= -.13643254E+02 F= -.14152912E+02 E0=.. EK= 0.50966E+00 SP= 0.00E+00 SK= 0.00E+00
3 T=  1336. E= -.13629241E+02 F= -.13974630E+02 E0=.. EK= 0.34539E+00 SP= 0.00E+00 SK= 0.00E+00
4 T=  1011. E= -.13624149E+02 F= -.13885486E+02 E0=.. EK= 0.26134E+00 SP= 0.00E+00 SK= 0.00E+00
5 T=  1307. E= -.13629772E+02 F= -.13967549E+02 E0=.. EK= 0.33778E+00 SP= 0.00E+00 SK= 0.00E+00
 ...  ...  ...
 ...  ...  ...
 ...  ...  ...
```

Start p4vasp:

```
> p4v [vasprun.xml]
```

Step 1.) Go to: Convergence/Energy

Step 2.) Update graph



System: ??? (vasprun.xml)

Selection:

OK

Further things to try

- How does the energy change when you decrease `SIGMA` to 0.01 in the INCAR file starting from O atom? Why?
- Try to copy CONTCAR to POSCAR after running the example O dimer. Why is the calculation so fast?
- Try to play with the parameter `POTIM` for the example O dimer. What is the optimal value ?
- What is the reason for the imaginary frequency in the example CO vibration. Does the behavior improve when the step width (smaller or larger) is changed. Also try to improve the precession to which the ground state is converged (`EDIFF=1E-5`). What happens if the accuracy of the calculations is improved (`PREC=Accurate`).
- Try to use the conjugate gradient algorithm to the H_2O molecule (example H2O).
- Calculate the vibrational frequencies of the H_2O molecule (example H2O) after relaxation (example H2Ovib). Why does one find 3 modes that have small frequencies. `EDIFF=1E-5` gives much improved results than `EDIFF=1E-4`, can you reproduce this behavior.

Bulk Systems

Examples:

- fcc Si and cd Si
- fcc Ni

Tasks:

- Equilibrium volume & structure
- Density-Of-States
- Bandstructure

Equilibrium volume of fcc Si (ex.: fcc Si)

- INCAR:

`System = fcc Si`	
`ISTART = 0`	wave functions initialized with random numbers
`ICHARGE = 2`	charge density starts with density of “overlapping atoms”
`ENCUT = 240`	energy cutoff: 240 eV (see POTCAR)
`ISMEAR = 0 ; SIGMA = 0.1`	

- KPOINTS:

`K-Points`	Header (comment)
`0`	$N_k=0$: automatic mesh generation
`Monkhorst-Pack`	Monkhorst-Pack grid
`11 11 11`	# of subdivisions N_i along $\vec{b}_i$ (odd: centered on Γ)
`0. 0. 0.`	Optionally shift the mesh (s_i)

Results in 56 **k**-points in the IBZ

Equilibrium volume of fcc Si (ex.: fcc Si)

- POSCAR:

fcc Si:	Header (comment)
3.9	lattice constant
0.5 0.5 0.0 0.0 0.5 0.5 0.5 0.0 0.5	fcc lattice vectors
1	Number of atoms for each species
cartesian	Positions in cartesian coordinates
0 0 0	

How can one calculate the groundstate volume?

- Calculate the total energy for different lattice parameters
- Fit to some ”Equation-Of-State” to obtain the equilibrium volume

Equilibrium volume of fcc Si (ex.: fcc Si)

Automated volume scan (by means of a shell script): loop.sh

```
#!/bin/bash
vasp_std=”mpirun -np 8 some-vasp-executabel”

rm WAVECAR SUMMARY.fcc

for i in  3.5 3.6 3.7 3.8 3.9 4.0 4.1 4.2 4.3 ; do
cat >POSCAR <<!
fcc:
   $i
 0.5 0.5 0.0
 0.0 0.5 0.5
 0.5 0.0 0.5
   1
cartesian
0 0 0
!
echo "a= $i"

$vasp_std

E=`awk '/F=/ {print $0}' OSZICAR` ; echo $i $E
>>SUMMARY.fcc
done
cat SUMMARY.fcc
```

loop.sh:

- Unix bash script
- Use lattice parameters from 3.5 to 4.3 Å
- Results written to SUMMARY.fcc

Equilibrium volume of fcc Si (ex.: fcc Si)

- SUMMARY.fcc: Total energy vs. lattice parameter:

```
3.5 1 F= -.44256712E+01 E0= -.44233993E+01 d E =-.454388E-02
3.6 1 F= -.46614699E+01 E0= -.46600410E+01 d E =-.285796E-02
3.7 1 F= -.47979864E+01 E0= -.47959298E+01 d E =-.411323E-02
3.8 1 F= -.48645042E+01 E0= -.48630063E+01 d E =-.299564E-02
3.9 1 F= -.48773847E+01 E0= -.48758538E+01 d E =-.306176E-02
4.0 1 F= -.48487436E+01 E0= -.48481092E+01 d E =-.126878E-02
4.1 1 F= -.47852634E+01 E0= -.47844854E+01 d E =-.155599E-02
4.2 1 F= -.46936947E+01 E0= -.46922530E+01 d E =-.288339E-02
4.3 1 F= -.45831167E+01 E0= -.45811837E+01 d E =-.386598E-02
```

- The equilibrium lattice constant (minimum in the total energy) is found at roughly: 3.9 Å.

  Adjust your POSCAR file to reflect this, and rerun VASP.

  N.B.: Keep your CHGCAR file from this run, we will need it in the following examples.

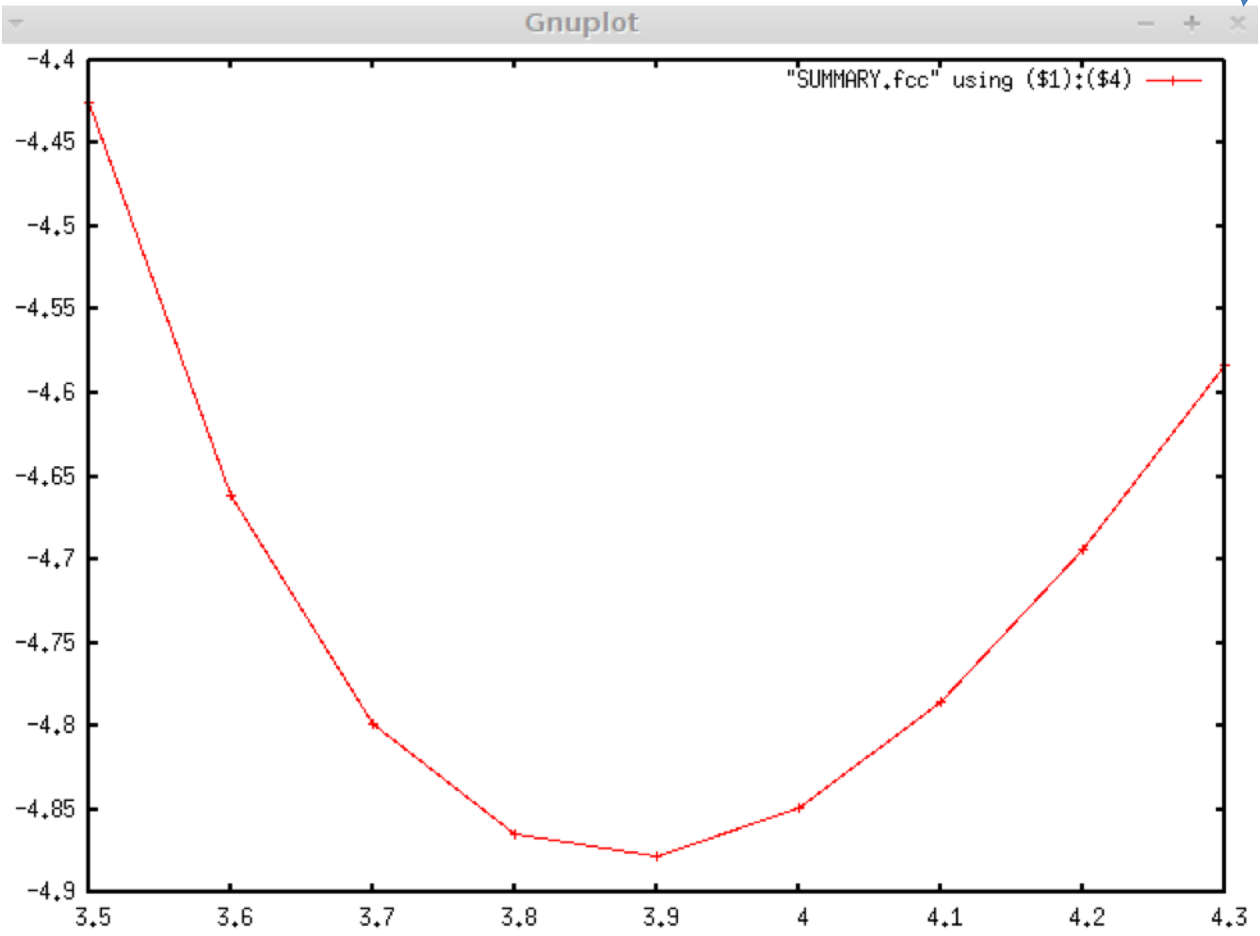
```
fcc Si:

3.9

0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5

1

cartesian

0 0 0
```

Equilibrium volume of fcc Si (ex.: fcc Si)

A quick look at the results?

```
>gnuplot
      gnuplot> plot "SUMMARY.fcc" using ($1):($4) w lp
      gnuplot> exit
```

“kill the window with”



Density-Of-States of fcc Si (ex.: fcc Si DOS)

To compute the density-of-states (DOS) there are two possibilities:

I. Perform a static (`NSW=0 ; IBRION=-1`) self-consistent calculation → the DOS is written to the DOSCAR file

II. For a large system:
   1. Perform a self-consisten calculation with a “small” number of **k**-points.
   2. For the DOS: increase the **k**-point sampling density, and set `ICHARG=11`, *i.e.*, read in the charge density (CHGCAR) from the previous self-consistent run, and keep it fixed.

- For `ICHARG=11` all k-point are treated independently
- Charge density and potential are kept fixed
- Used to compute band structure (as well)

Density-Of-States of fcc Si (ex.: fcc Si DOS)

- INCAR:

`System = fcc Si`	
`ICHARGE = 11`	Read charge density from previous run, and keep it fixed during this calculation
`ENCUT = 240`	energy cutoff: 240 eV (see POTCAR)
`ISMEAR = -5`	Use the tetrahedron method with Blöchl corrections

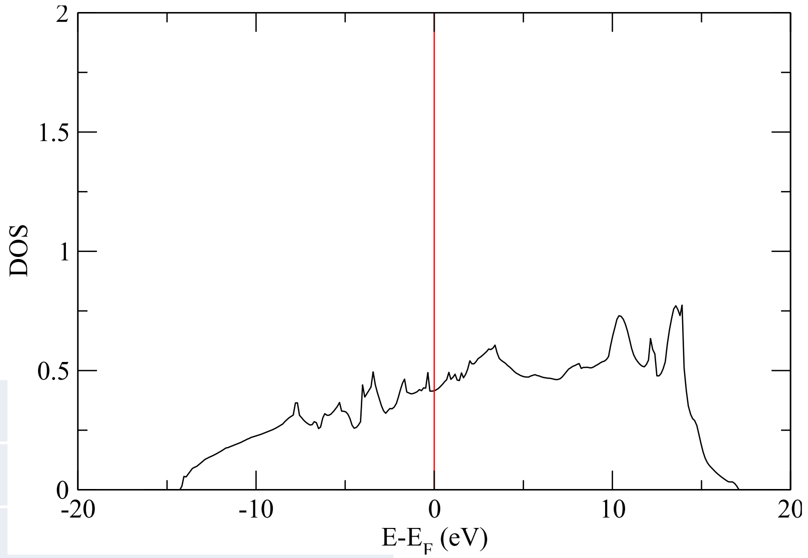
N.B.: copy the self-consistent charge density of the fcc Si example to your current working directory!

You must do this, otherwise will not be able to read the CHGCAR file, and will terminate.

N.B.: Uses the tetrahedron-method.

- KPOINTS:

`K-Points`	Header (comment)
`0`	N_k=0: automatic mesh generation
`Monkhorst-Pack`	Monkhorst-Pack grid
`21 21 21`	# of subdivisions N_i along $\vec{b}_i$ (odd: centered on Γ)
`0. 0. 0.`	Optionally shift the mesh (s_i)

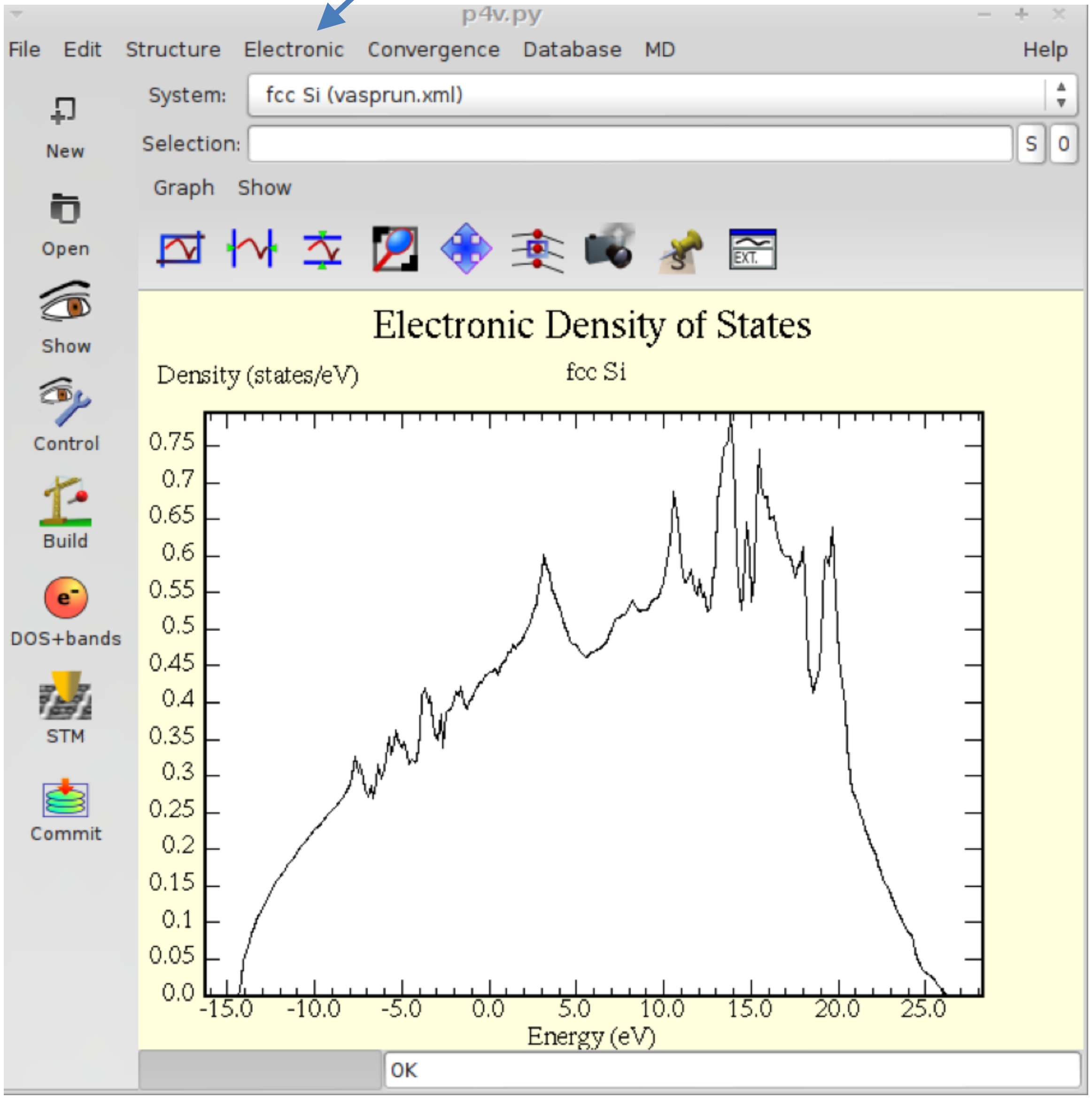


Density-Of-States of fcc Si (ex.: fcc Si DOS)

Start p4vasp:

```
> p4v [vasprun.xml]
```

Go to: Electronic/DOS+bands



System: fcc Si (vasprun.xml)

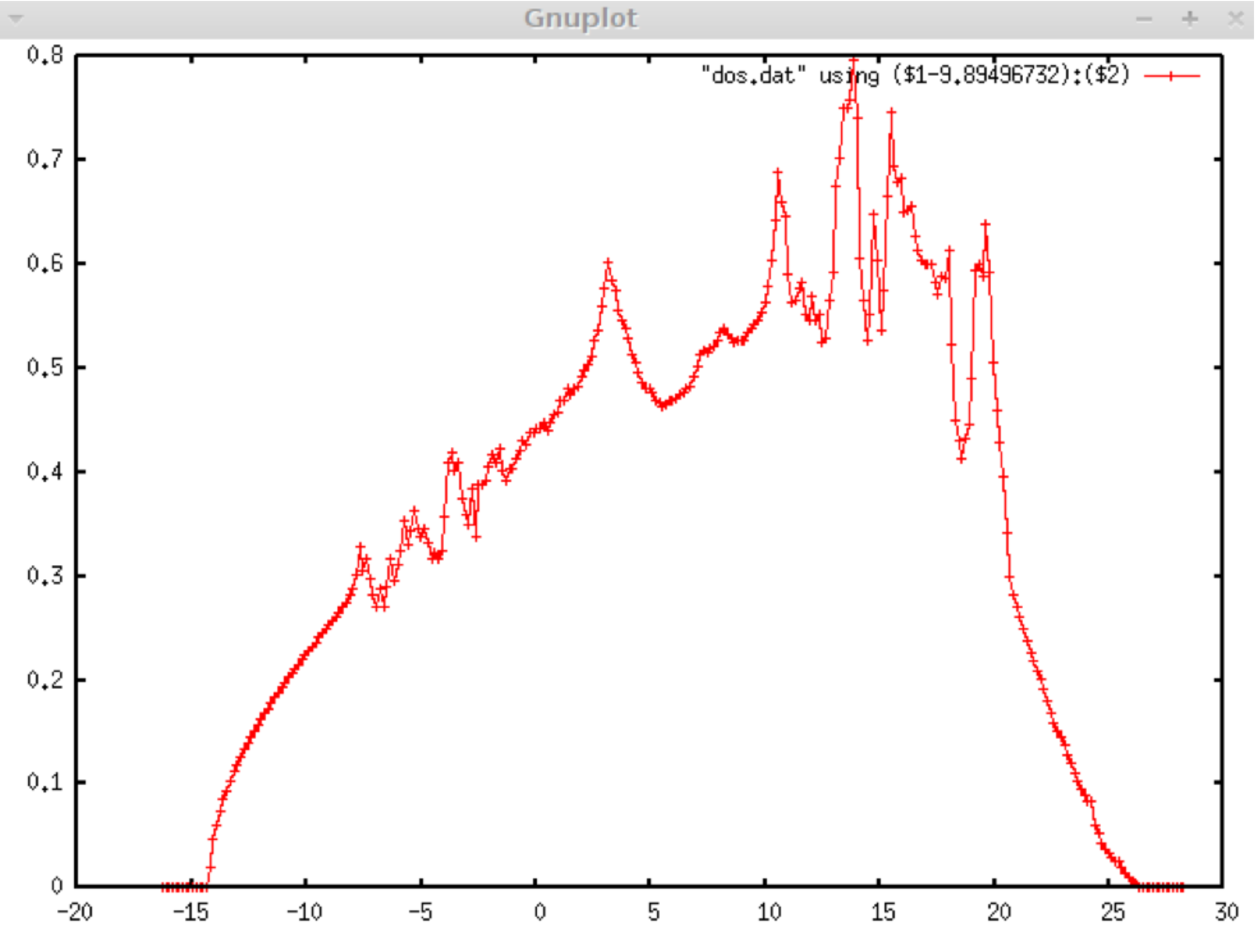
Selection:

OK

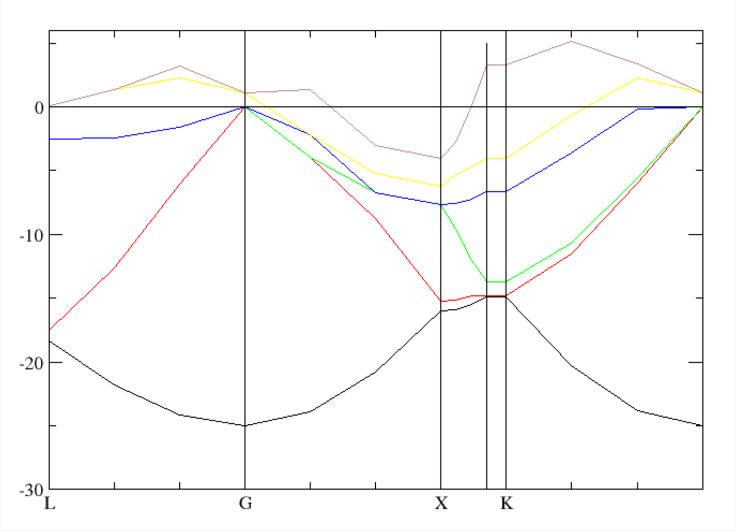
Density-Of-States of fcc Si (ex.: fcc Si DOS)

Or use gnuplot for a quick look:

```
> ./plotdos.sh
```



Bandstructure of fcc Si (ex.: fcc Si band)

L-G-X-U K-G	Header (comment)
10	10 points per line segment
line	Switch for bandstructure
reciprocal	begin/end-points in reciprocal coordinates
0.50000 0.50000 0.50000 1 0.00000 0.00000 0.00000 1	L-point G-point 
0.00000 0.00000 0.00000 1 0.00000 0.50000 0.50000 1	G-point X-point
0.00000 0.50000 0.50000 1 0.25000 0.62500 0.62500 1	X-point U-point
0.37500 0.75000 0.37500 1 0.00000 0.00000 0.00000 1	K-point G-point
	All points are weighted ″× 1″

N.B.: copy the self-consistent charge density of the previous example (fcc Si DOS) to your current working directory.

You must do this otherwise VASP cannot read the CHGCAR file, and will terminate.

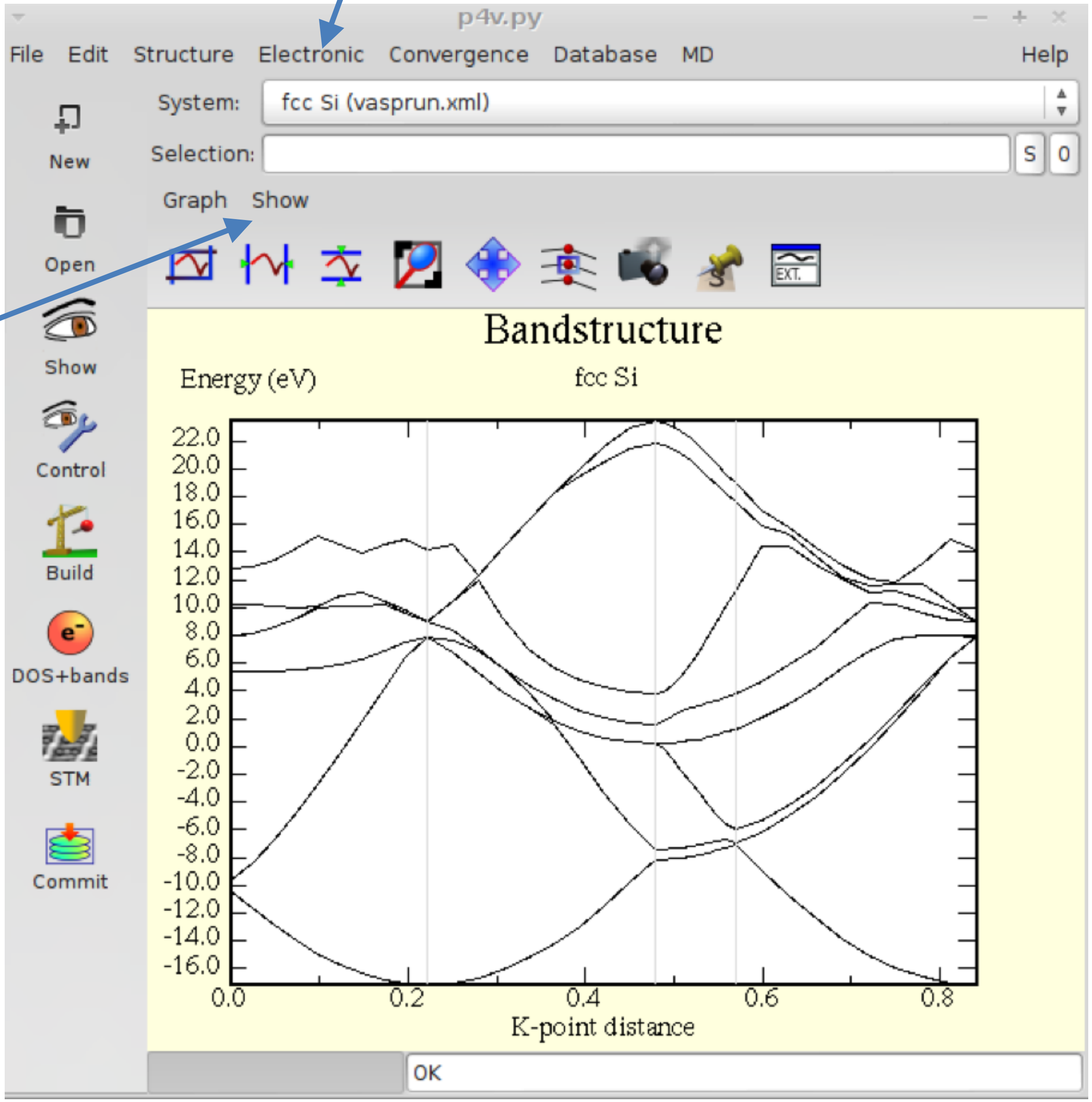
Bandstructure of fcc Si (ex.: fcc Si band)

Start p4vasp:

```
> p4v [vasprun.xml]
```

Step 1.) Go to: Electronic/DOS+bands

Step 2.) Go to: Show/Bands



System: fcc Si (vasprun.xml)

Selection:

Cubic-diamond Si (ex.: cd Si)

To do:

1. Determine the equilibrium lattice constant/volume
2. Calculate DOS (at equilibrium volume)
3. Compute the bandstructure (at equilibrium volume)

Job scripts:

1. loop.sh
2. dos.sh
3. band.sh

Visualization: as in the examples fcc Si, fcc Si DOS, and fcc Si band.

N.B.: Have a look at the README file, and take a look at what the scripts do!

Equilibrium volume of cd-Si (ex.: cd Si)

```
5.2 1 F= -.10528151E+02 E0= -.10528137E+02 d E =-.274709E-04
5.3 1 F= -.10713281E+02 E0= -.10713280E+02 d E =-.218410E-05
5.4 1 F= -.10806685E+02 E0= -.10806685E+02 d E =-.114401E-06
5.5 1 F= -.10823039E+02 E0= -.10823039E+02 d E =-.429842E-08
5.6 1 F= -.10775102E+02 E0= -.10775102E+02 d E =-.204668E-09
5.7 1 F= -.10673578E+02 E0= -.10673578E+02 d E =-.112715E-10
5.8 1 F= -.10528393E+02 E0= -.10528393E+02 d E =-.552513E-11
```

SUMMARY.diamond:

- Energy vs. lattice parameter (loop.sh): *a* = 5.465 Å
- For DOS and band-structure, rounded to *a* = 5.5 Å

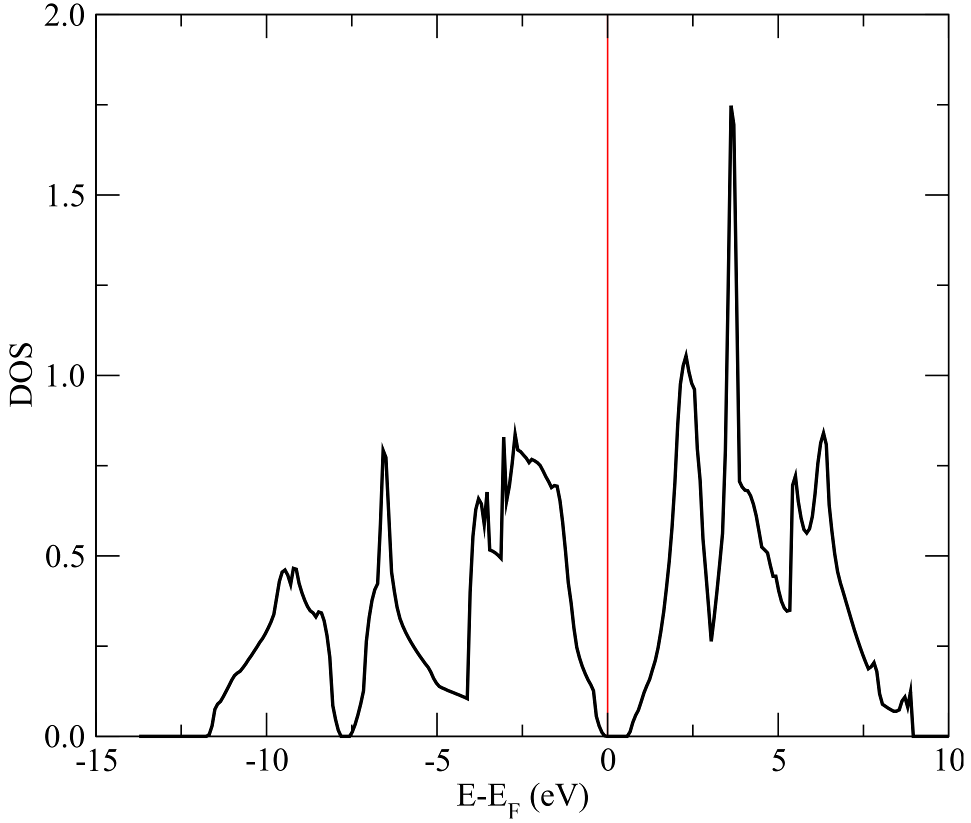
cubic diamond	Header (comment)
5.5	lattice constant
0.5 0.5 0.0 0.5 0.0 0.5 0.5 0.5 0.0	fcc lattice vectors
2	Number of atoms for each species
Direct	Positions in direct coordinates
-0.125 -0.125 -0.125 0.125 0.125 0.125	

POSCAR:

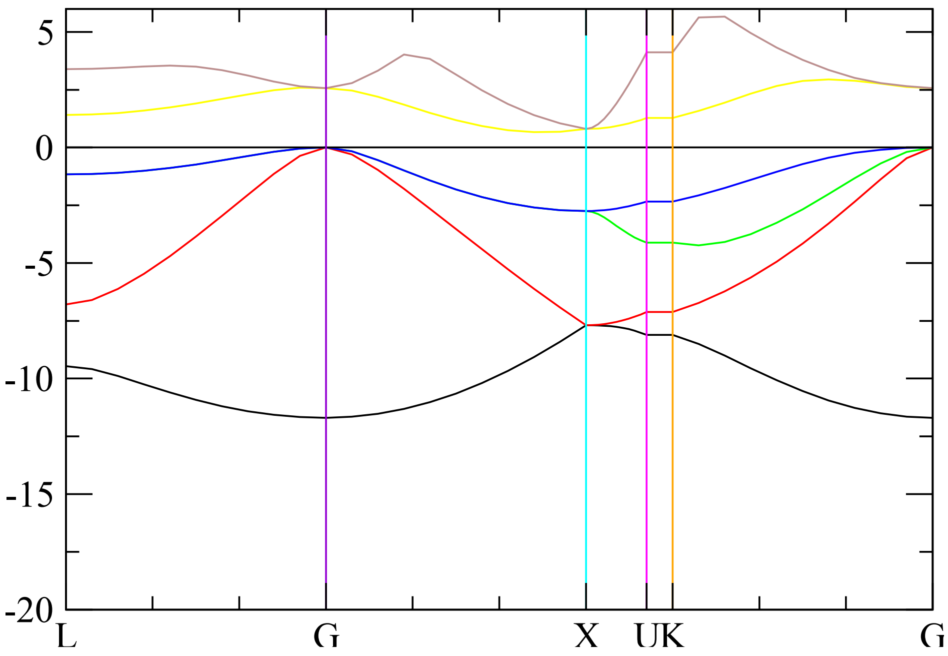
- fcc cell
- 2 atoms in cell

DOS and bandstructure of cd-Si (ex.: cd Si)

- DOS



- Bandstructure



“Fat” bands (ex.: cd Si)

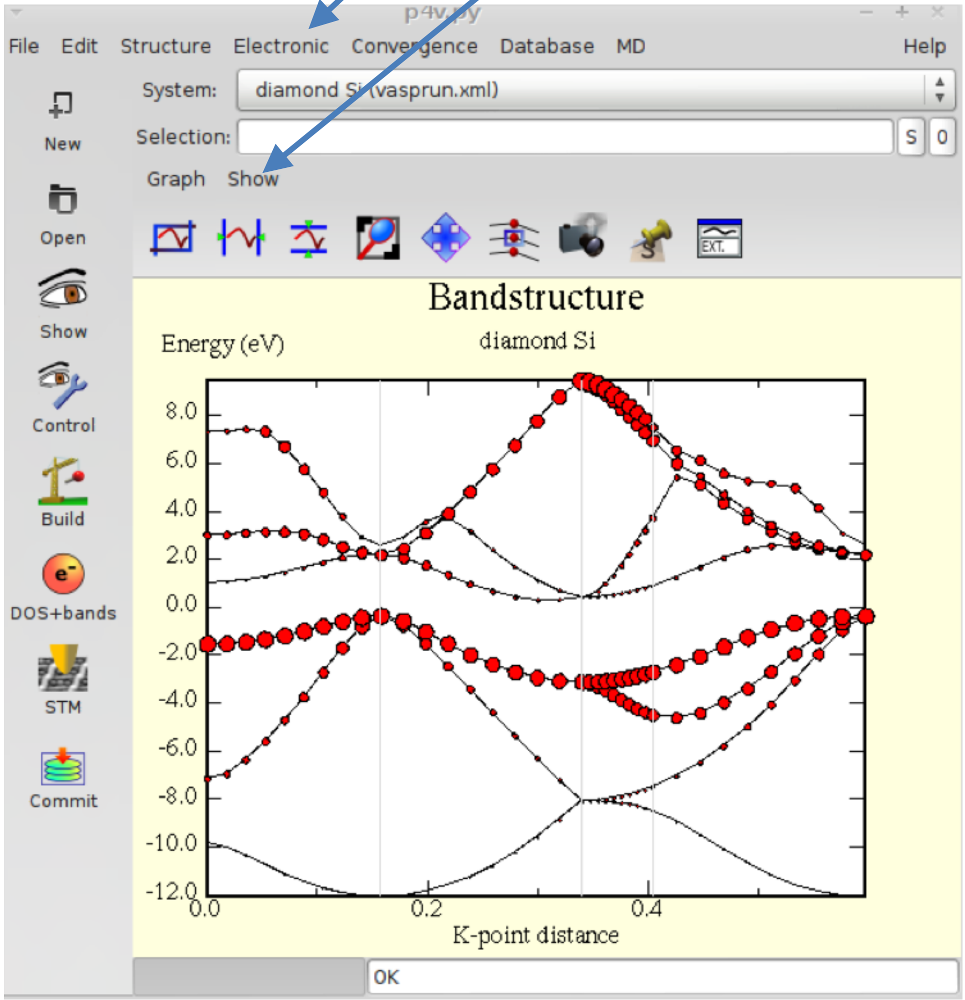
Start p4vasp:
> p4v [vasprun.xml]

Step 1.) Go to: Electronic/Local DOS+bands control

Step 2.) Go to: Show/Bands

Step 3.) select atoms: “all”, “Si”, “1”, “2”, ...

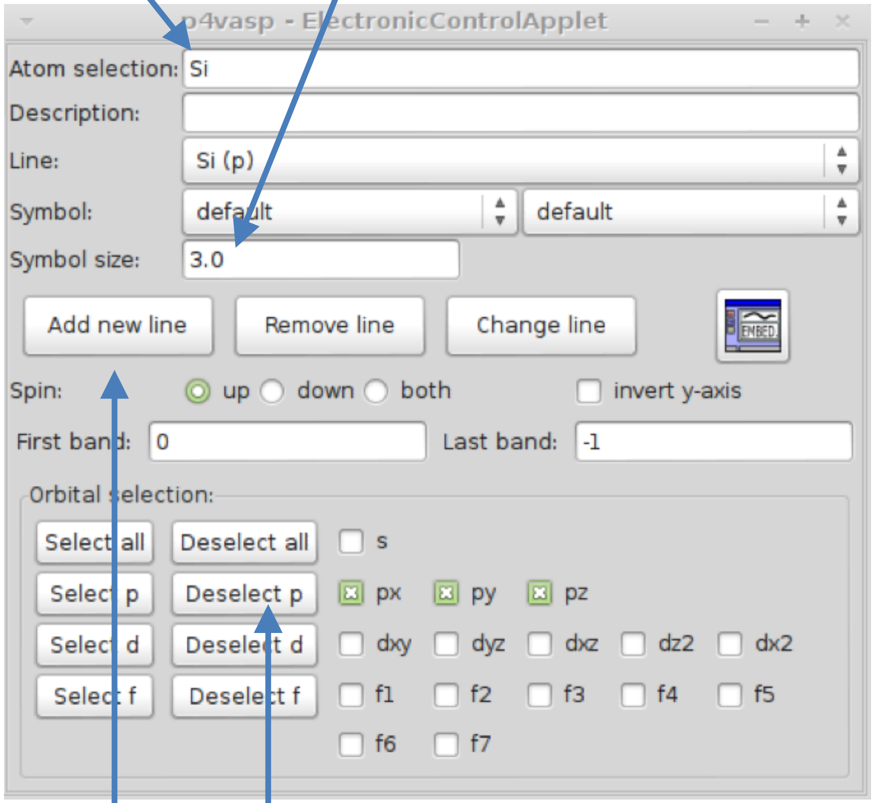
Step 4.) Adjust symbol size



System: diamond Si (vasprun.xml)

Selection:

OK



Atom selection: Si

Description:

Line: Si (p)

Symbol: default | default

Symbol size: 3.0

Spin: ● up ○ down ○ both ☐ invert y-axis

First band: 0 Last band: -1

☐ s
☒ px ☒ py ☒ pz
☐ dxy ☐ dyz ☐ dxz ☐ dz2 ☐ dx2
☐ f1 ☐ f2 ☐ f3 ☐ f4 ☐ f5
☐ f6 ☐ f7

Step 5.) Select orbital character

Step 6.) and “add new line”

Volume relaxation of cd-Si (ex.: cd Si vol relax)

To determine the equilibrium volume we can:

- fit the energy over a certain volume range to an equation of states (e.g. the Murnaghan equation of states).

Alternatively, we will now try:

- Relaxing the structure with VASP
  - `IBRION = 2` conjugate gradient algorithm
  - `ISIF = 3` change internal coordinates, and cell shape & volume

`System = diamond Si`	
`ISMEAR = 0` `SIGMA = 0.1`	Gaussian smearing Smearing width $\sigma = 0.1$ eV
`ENMAX = 400`	energy cutoff: 400 eV

`IBRION = 2`
`ISIF = 3`
`NSW = 15`
	Use conjugate gradient algorithm
	Change internal coord., and cell shape&volume
	Maximum number of relaxation steps

`EDIFF = 0.1E-5`	Convergence of electronic system: changes in total energy < 10^{-6}
`EDIFFG = -0.001`	Convergence of structural relaxation: forces on ions < 0.001 eV/Å

Volume relaxation of cd-Si (ex.: cd Si vol relax)

OUTCAR:

```
  ---------------------------------------------------------------------------------------
   Total        0.00155     0.00155     0.00155    -0.00000    -0.00000     0.00000
   in kB        0.06056     0.06056     0.06056    -0.00000    -0.00000     0.00000
   external pressure =        0.06 kB  Pullay stress =        0.00 kB


  VOLUME and BASIS-vectors are now :
  -------------------------------------------------------------------------------
   energy-cutoff  :      400.00
   volume of cell :       40.88
       direct lattice vectors                 reciprocal lattice vectors
      0.000000000  2.734185321  2.734185321    -0.182869828  0.182869828  0.182869828
      2.734185321  0.000000000  2.734185321     0.182869828 -0.182869828  0.182869828
      2.734185321  2.734185321  0.000000000     0.182869828  0.182869828 -0.182869828
```

- From equation of states: *a* = 5.4687 Å
  (volume scan + Murhaghan EOS, using `ENMAX = 400` eV!)
- From the previous relaxation we find: a = 5.4684 Å
- The difference can be due to Pulay stress
  (especially when the relaxation starts far away from equilibrium).
  - increase the plane wave cutoff energy by at least 30%
    (here we used `ENMAX=400` instead of 240!)
  - use small `EDIFF`

Volume relaxation of cd-Si (ex.: cd Si vol relax)

- Calculation of the equilibrium volume "at constant cutoff":
  - fit the energy over a certain volume range to an equation of states
  - when internal degrees of freedom exist (e.g. c/a), the structure must be optimized at each volume:

`IBRION = 2` conjugate gradient algorithm

`NSW = 10` e.g. 10 ionic steps

`ISIF = 4` change internal coord. and cell shape

- Simpler, but less reliable: calculate eq. volume "at constant basis set":
  - relax all degrees of freedom including volume:

`ISIF = 3` change internal coord., and cell shape & volume

  - mind Pulay stress problem: increase plane wave cutoff energy by 25-30 % when the volume is allowed to change

Ionic relaxation in cd-Si (ex.: cd Si ion relax)

INCAR:

System = diamond Si	
ISTART = 0 ICHARG = 2	Initialize wave functions with random numbers Initial charge density: overlapping atomic charge densities
ISMEAR = 0 SIGMA = 0.1	Gaussian smearing Smearing width $\sigma = 0.1$ eV
ENMAX = 240	energy cutoff: 240 eV
IBRION = 2 ISIF = 2 NSW = 10	Use conjugate gradient algorithm Change internal coordinates only Maximum number of relaxation steps
EDIFFG = -0.0001	Convergence of structural relaxation: forces on ions < 0.0001 eV/Å

Ionic relaxation in cd-Si (ex.: cd Si ion relax)

POSCAR:

- changed *z* coordinates: from 0.125 to 0.130
- “cubic“ diamond structure → cubic symmetry is broken.

cubic diamond	Header (comment)
5.5	lattice constant
0.5 0.5 0.0 0.5 0.0 0.5 0.5 0.5 0.0	fcc lattice vectors
2	Number of atoms for each species
Direct	Positions in direct coordinates
-0.125 -0.125 -0.130 0.125 0.125 0.130	

OUTCAR: after 10 steps

```
POSITION                                          TOTAL-FORCE (eV/Angst)
---------------------------------------------------------------------------------
     4.81253      4.81253      4.81250      -0.000724     -0.000724     -0.000031
     0.68747      0.68747      0.68750       0.000724      0.000724      0.000031
---------------------------------------------------------------------------------
   total drift:                              0.000000      0.000000      0.000000
```

Ionic relaxation: general comments

- Files to watch during relaxations:
  - `stdout` (the "terminal") , each electronic step is written to the terminal
  - OSZICAR: a copy of the terminal output
  - OUTCAR: detailed information on every electronic and ionic step

- Other important files:
  - CONTCAR contains the structure of the last ionic step, i.e., the result of the relaxation (can be used to restart/continue a relaxation)
  - STOPCAR: can be created to stop a relaxation

fcc Ni (ex.: fcc Ni)

INCAR:

System = fcc Ni	
ISTART = 0 ICHARG = 2	Initialize wave functions with random numbers Initial charge density: overlapping atomic charge densities
ENMAX = 270	energy cutoff: 270 eV
ISMEAR = 1 SIGMA = 0.2	1st -order Methfessel-Paxton smearing (metallic system!) Smearing width $\sigma = 0.2$ eV
ISPIN = 2 MAGMOM = 1	Spin: Switch on spin-polarization Initial local magnetic moment of 1 μ_B

KPOINTS:

K-Points	Header (comment)
0	N_k=0: automatic mesh generation
Monkhorst-Pack	Monkhorst-Pack grid
11 11 11	# of subdivisions N_i along $\vec{b}_i$
0. 0. 0.	Optionally shift the mesh (s_i)

- Equally spaced mesh, yields 56 **k**-points in the IBZ
- Odd → centered at **Γ**

fcc Ni (ex.: fcc Ni)

To do:

1. Determine the equilibrium lattice constant/volume
2. Calculate DOS (at equilibrium volume)
3. Compute the bandstructure (at equilibrium volume)

Job scripts:

1. loop.sh
2. dos.sh
3. band.sh

Visualization: as in the examples fcc Si, fcc Si DOS, and fcc Si band.

But beware: there are separate spin-up and spin-down states!

N.B.: Have a look at the README file, and take a look at what the scripts do!

fcc Ni (ex.: fcc Ni)