Data analysis and Plotting

- Simulating STM images
- Bonding charge analysis
- Calculating surface energies

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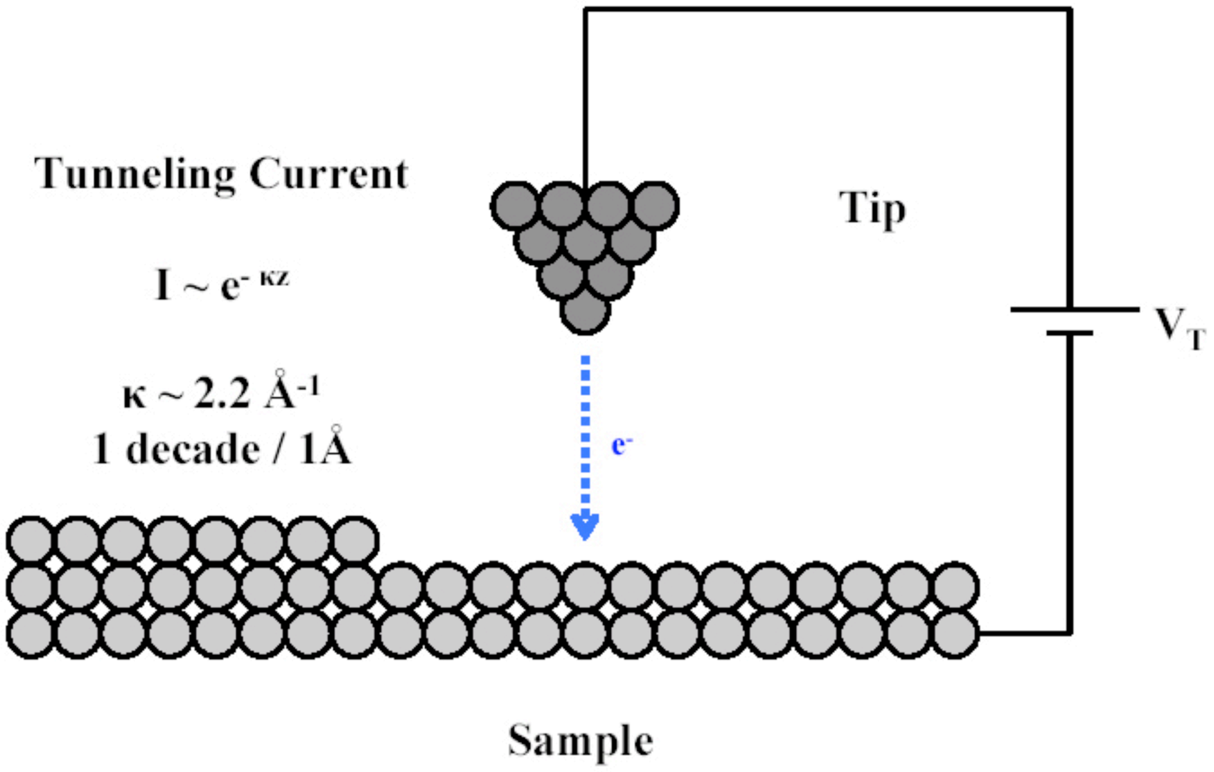
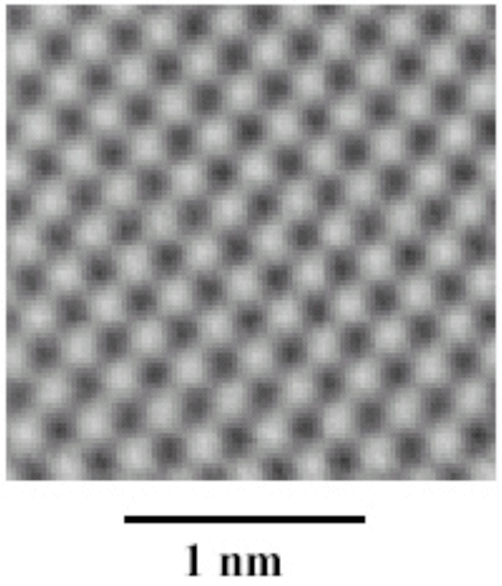
STM microscopy

(Binning and Rohrer, 1986 Nobel prize for Physics)





$$I = \frac{2\pi e}{\hbar}\sum_{\mu\nu} \overset{\textbf{\textit{probe}}}{f(E_\mu)}\,\underset{\textbf{\textit{surface}}}{[1 - f(E_\nu + eV)]} \times |M_{\mu\nu}|^2\delta(E_\mu - E_\nu)$$

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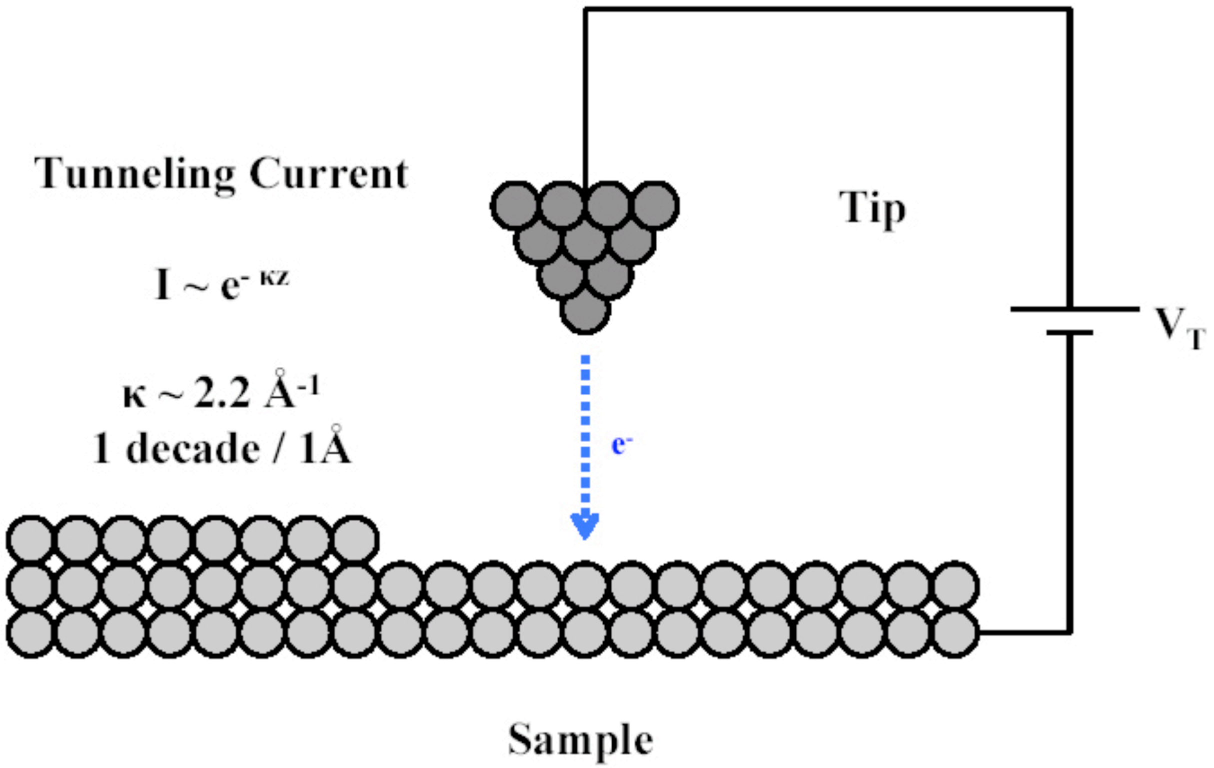

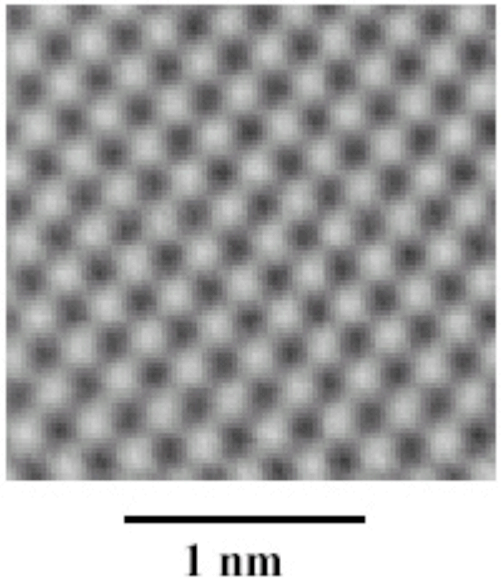

- Applied voltage between tip and sample results in electron tunneling
- Tunneling current exponential in the tip-sample distance
- General expression for the tunneling current between sample and tip

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Tersoff-Hamann

$$M_{\mu\nu} \propto \psi_\nu(\mathbf{r}_0)$$

$$I \propto \sum_\nu |\psi_\nu(\mathbf{r}_0)|^2 \, \delta(E_\nu - E_F)$$

$$D(\mathbf{r}, E_F) = \sum_\nu |\psi_\nu(\mathbf{r})|^2 \, \delta(E_\nu - E_F)$$

Tersoff & Hamann, PRL 50, 1998 (1983); PRB 31, 805 (1985)

Tersoff-Hamann

1) The tip is assumed to be a point source
2) The tip electronic structure is assumed to be described by s wave function -->

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… proportional to the local DOS of the surface at the Fermi energy

$$D(\mathbf{r}, E_F) = \sum_\nu |\psi_\nu(\mathbf{r})|^2\, \delta(E_\nu - E_F)$$

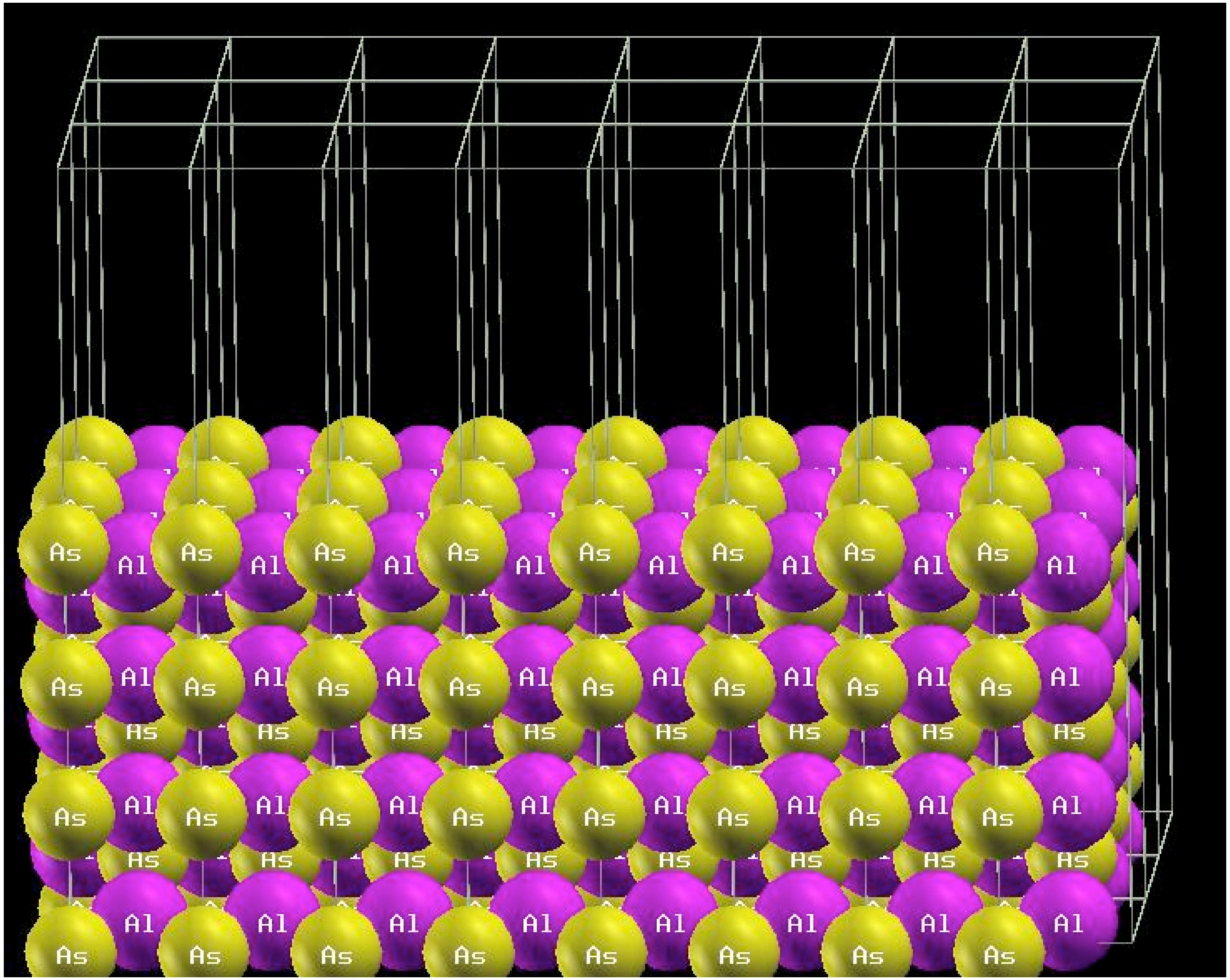
- In the limit of finite V and T=0 the current intensity is proportional to an integrated DOS:

$$\int_{E_F}^{E_F+V} \sum_\nu |\psi_\nu(\mathbf{r})|^2\, \delta(E_\nu - E)\mathrm{d}E$$

Tersoff & Hamann, PRL 50, 1998 (1983); PRB 31, 805 (1985)

Ex1: STM simulation

Simulate the STM image of the AlAs (110) surface



Ex1: STM simulation

1) Edit the file `run-alas.scf` and run the scf calculation of the AlAs(110) surface.

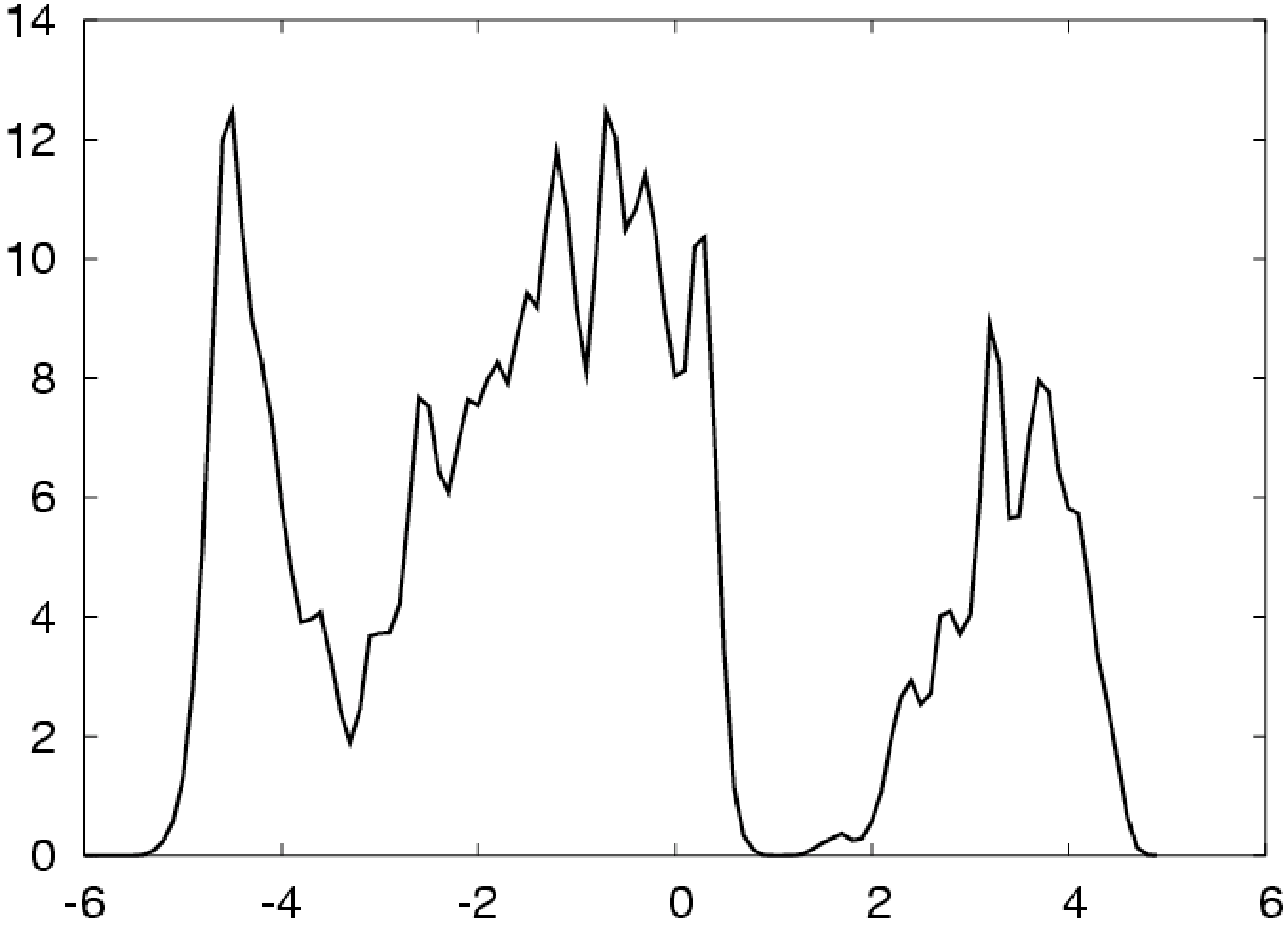
2) Edit the file `run-alas.nscf`: Increase the number of k points and run the corresponding nscf calculation.

3) Set up the input file (`run-alas.pp`) for postprocessing the data (`pp.x`).

```
 &inputpp
    prefix  = 'AlAs110'
    outdir='$TMP_DIR',
    filplot = 'AlAs-1.0'
    sample_bias=XXX,    <-- in Ry!
    plot_num= XXX
 /
 &plot
 /
```

Ex1: STM simulation

4) Positive values of bias sample occupied states (positive tip with respect to sample), while negative values of bias sample empty states (negative tip with respect to sample).



5) Run the postprocessing calculation: `run-alas.pp`

Ex1: STM simulation

6) Edit the file (**`run-alas.plot`**) for plotting the data (**`pp.x`**).

```
&inputpp
/
&plot
  nfile=xxxx
  filepp(1)='xxxx'
  weight(1)=xxx
  iflag=xx
  output_format=xx
  fileout='AlAs110-1.0.xsf'
/
```

7) Run the calculation **`run-alas.plot`**

8) Visualize the simulated STM image with XCrysDen

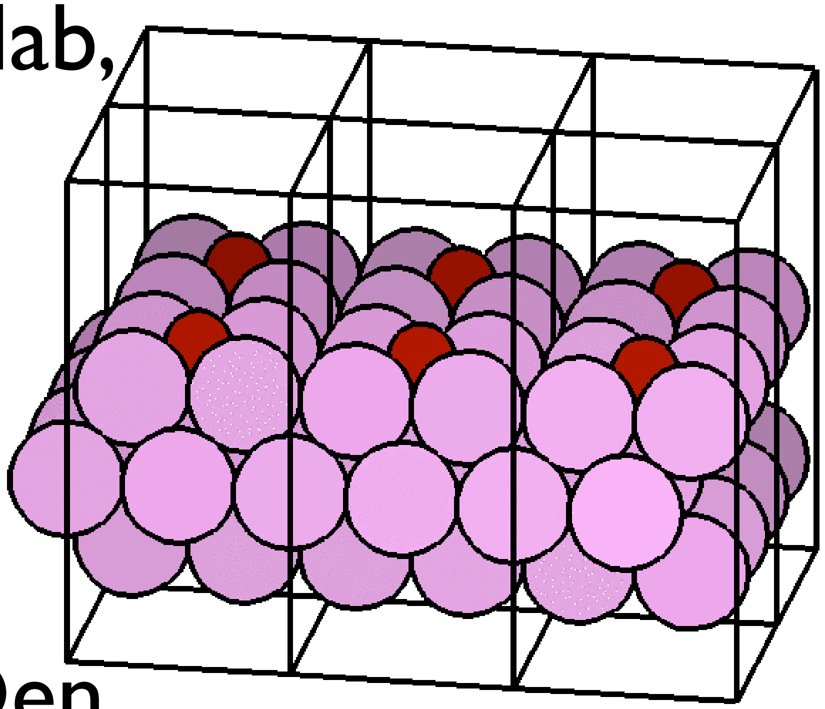
Ex2: bonding charge density

Calculate the bonding charge density of an O atom on the Al (001) surface

1) Inspect the following script run-Al-O-OAl-scf-pp

It contains the procedure for calculating the charge densities of three separated systems:

a) an O atom adsorbed on an Al(001) slab,
b) an Al(001) slab,
c) an O atom.



2) Run the script

3) Visualize the crystal structures with XCrysDen

4) Compare the atomic coordinates of the O atom in the file `O.scf.out` with those in `OAl.scf.out`.

Ex2: bonding charge density

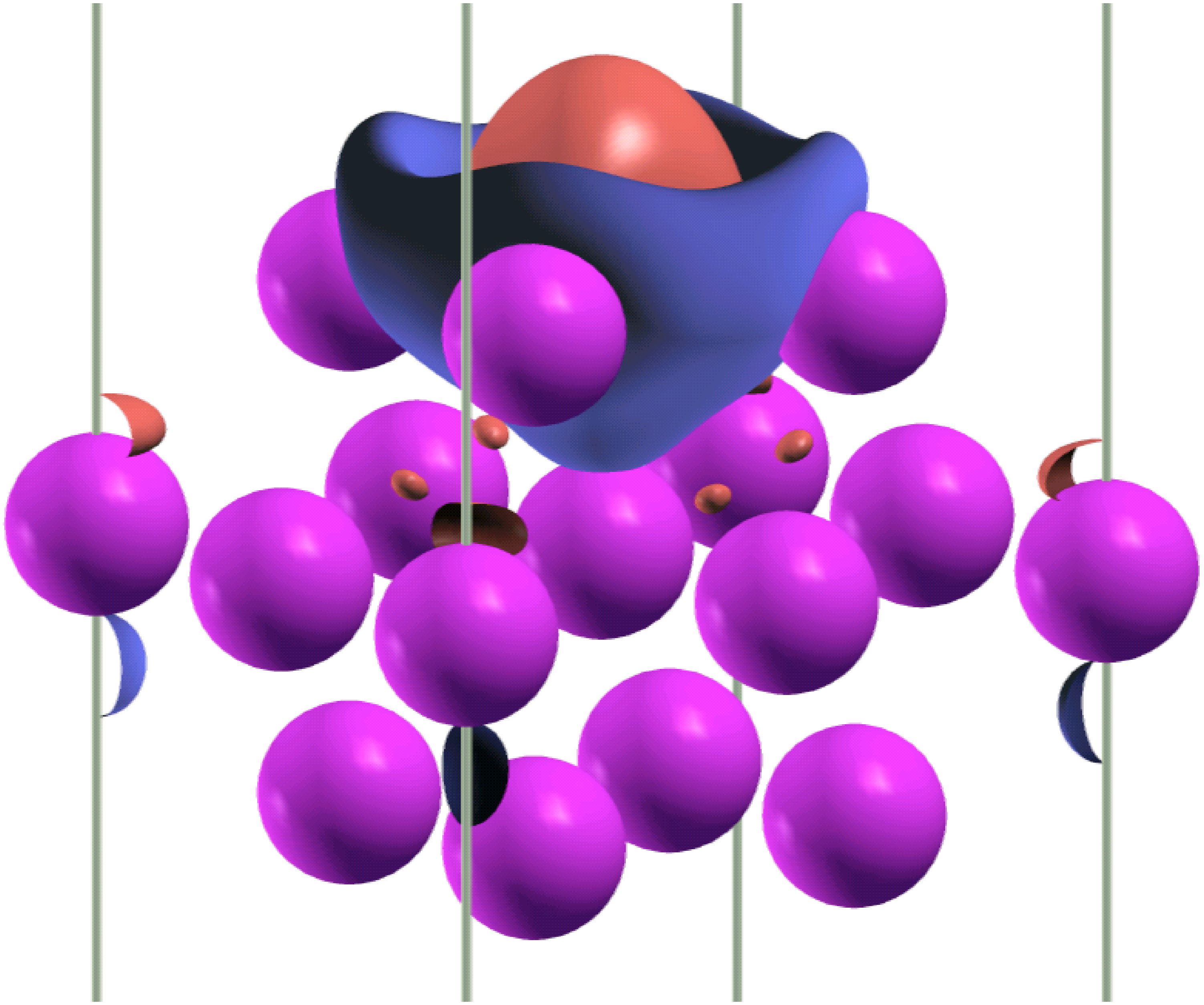
5) Set up an input file (**`run-pp`**) for the postprocessing program **`pp.x`**. The task is to subtract the charge densities of the Al(001) slab and of the O atom from the that one of the complete system O/Al(001

```
&inputpp
  nfile=xx
  filepp(1)='???', weight(1)=???
  filepp(2)='???', weight(2)=???
  filepp(3)='???', weight(3)=???
  iflag=xx
  plot_out=xx
  output_format=xx
  fileout='OAl.chdensDIFF.xsf'
/
```

Ex2: bonding charge density

6) Run the script **`run-pp`**

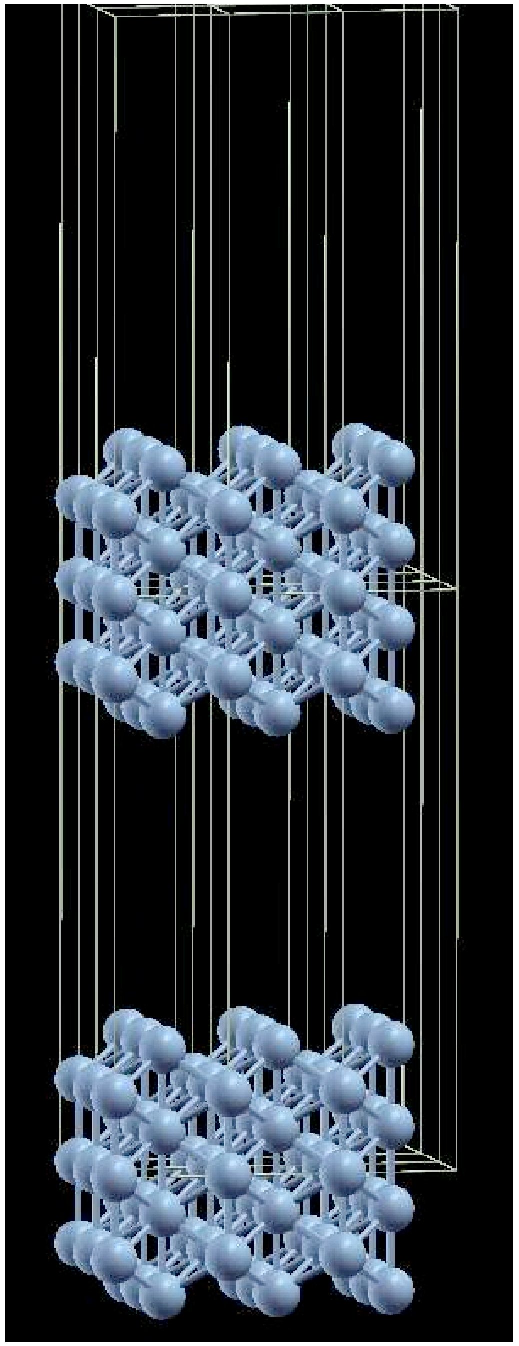
7) Visualize the resulting bonding charge density with XCrysDen



Ex3: surface energy

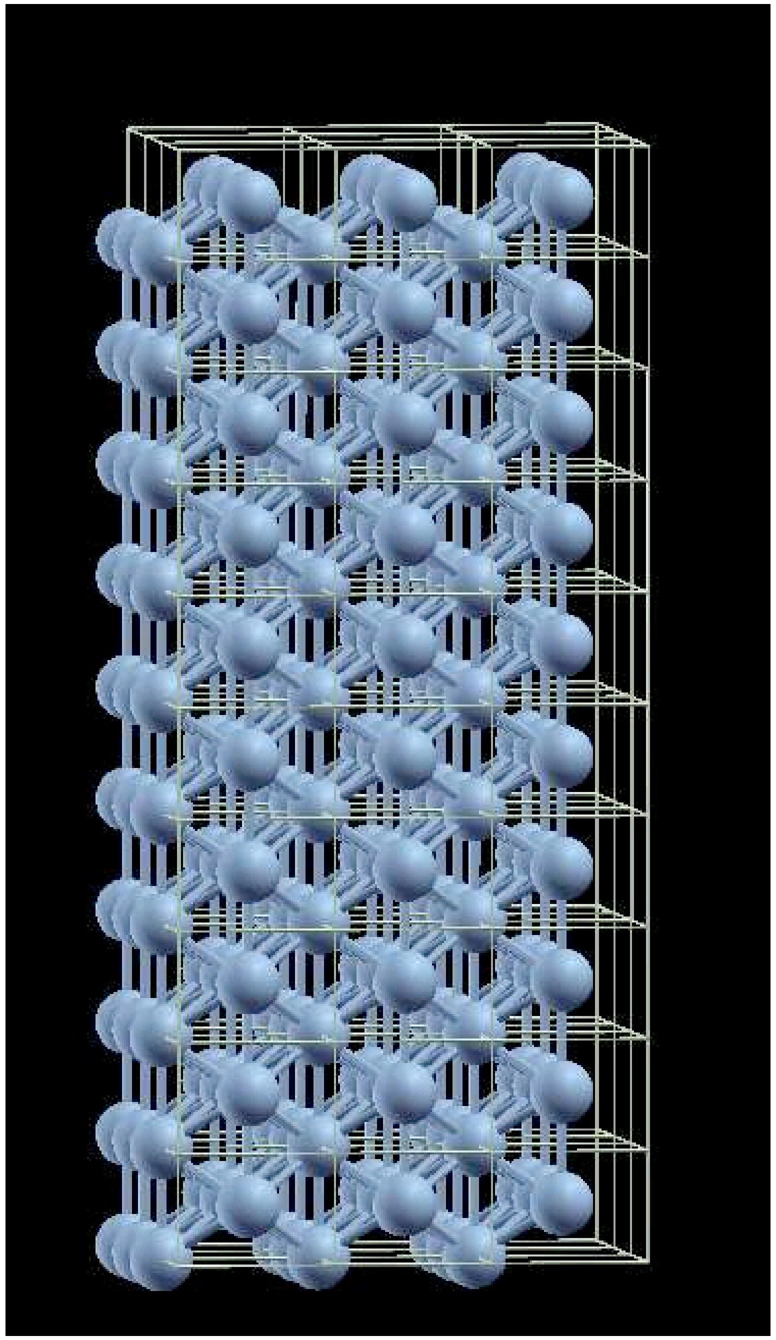
The surface energy of single component systems can be defined as

$$\gamma = \frac{1}{2A}\left(E^S - E^B\right)$$



- **Error cancellation:** Calculate E^S and E^B with the same computational parameters (basis set size, k-point mesh, smearing, …)

- **Convergence:** Check convergence of with respect to computational parameters and supercell model:
  - k-point mesh
  - cell thickness
  - vacuum thickness



Ex3: surface energy

Calculate the surface energy of the Cu(001) surface

$$\gamma = \frac{1}{2A}\left(E^S - E^B\right)$$

1) Model the Cu(001) surface with a tetragonal supercell slab having 4 atomic layers. Calculate E(slab).

2) Model the Cu bulk with a tetragonal supercell slab having 4 atomic layers. (Can you devise a more clever way of doing this calculation? Think at the k-point folding explored this morning ...) Calculate E(bulk)

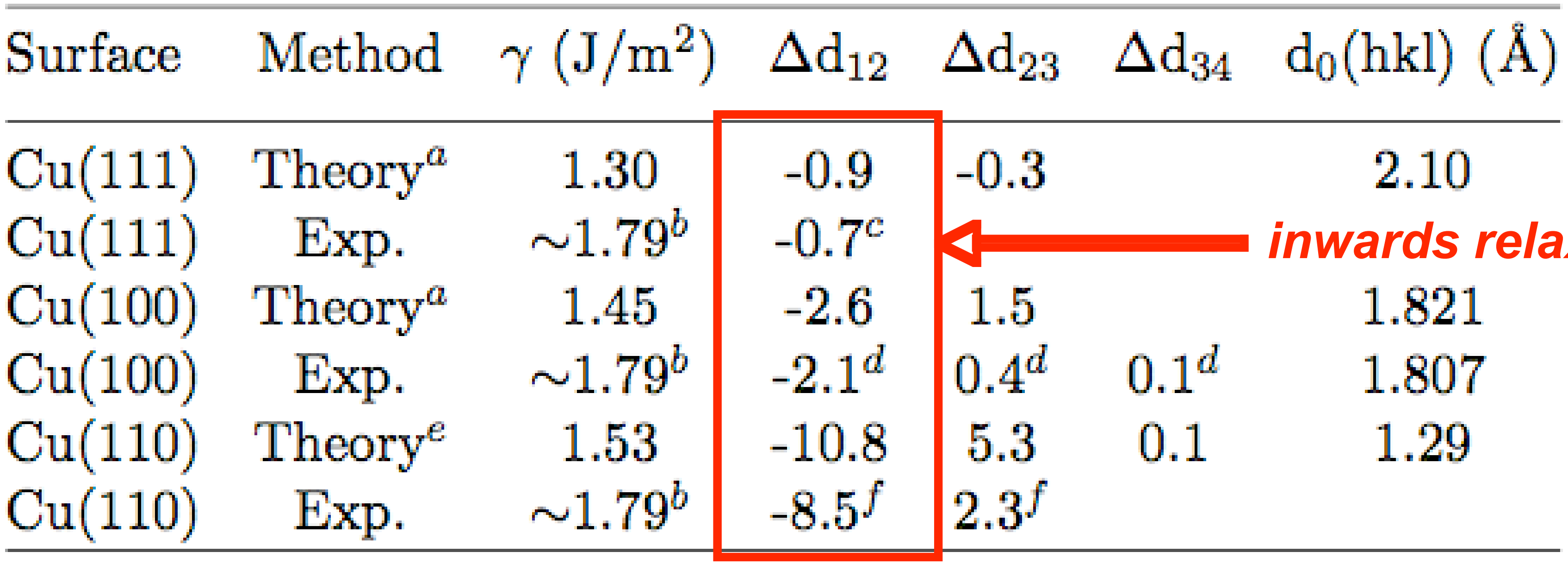
3) Calculate the total surface area 2A (where A is the area of each supercell side).

4) Calculate the surface energy.

Ex3: surface energy

5) Increase the number of layers in the slab (keeping the same vacuum distance) and check the convergency of the surface energy.

6) Compare with the literature and experiment:



Surface	Method	γ (J/m^2)	Δd_{12}	Δd_{23}	Δd_{34}	$d_0(hkl)$ (Å)
Cu(111)	Theory[a]	1.30	-0.9	-0.3		2.10
Cu(111)	Exp.	$\sim$1.79[b]	-0.7[c]			
Cu(100)	Theory[a]	1.45	-2.6	1.5		1.821
Cu(100)	Exp.	$\sim$1.79[b]	-2.1[d]	0.4[d]	0.1[d]	1.807
Cu(110)	Theory[e]	1.53	-10.8	5.3	0.1	1.29
Cu(110)	Exp.	$\sim$1.79[b]	-8.5[f]	2.3[f]		

inwards relaxation