CAMd
Center for Atomic-scale Materials Design

Atomic Simulation Environment

Souheil Saadi
saadi@fysik.dtu.dk
Thomas Olsen
tolsen@fysik.dtu.dk
Jens Jørgen Mortensen
jensj@fysik.dtu.dk
Ask Hjorth Larsen
askhl@fysik.dtu.dk

Atomic Simulation Environment

Toolbox for :

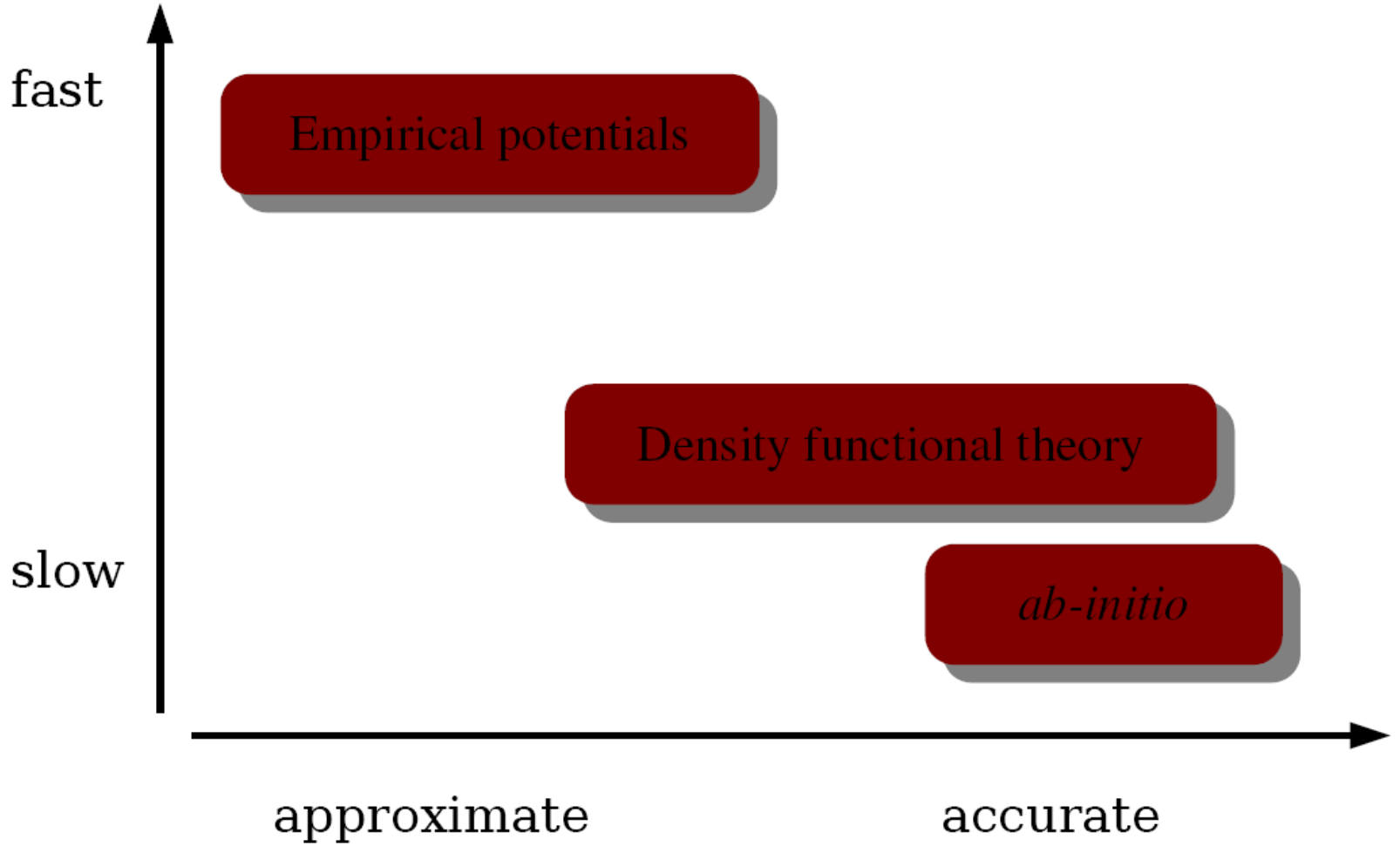
- Building atomic structures
- Molecular Dynamics
- Structure optimization
- Analysis
- Interface to several calculator codes: GPAW, ASAP, Dacapo...

The Python programming language

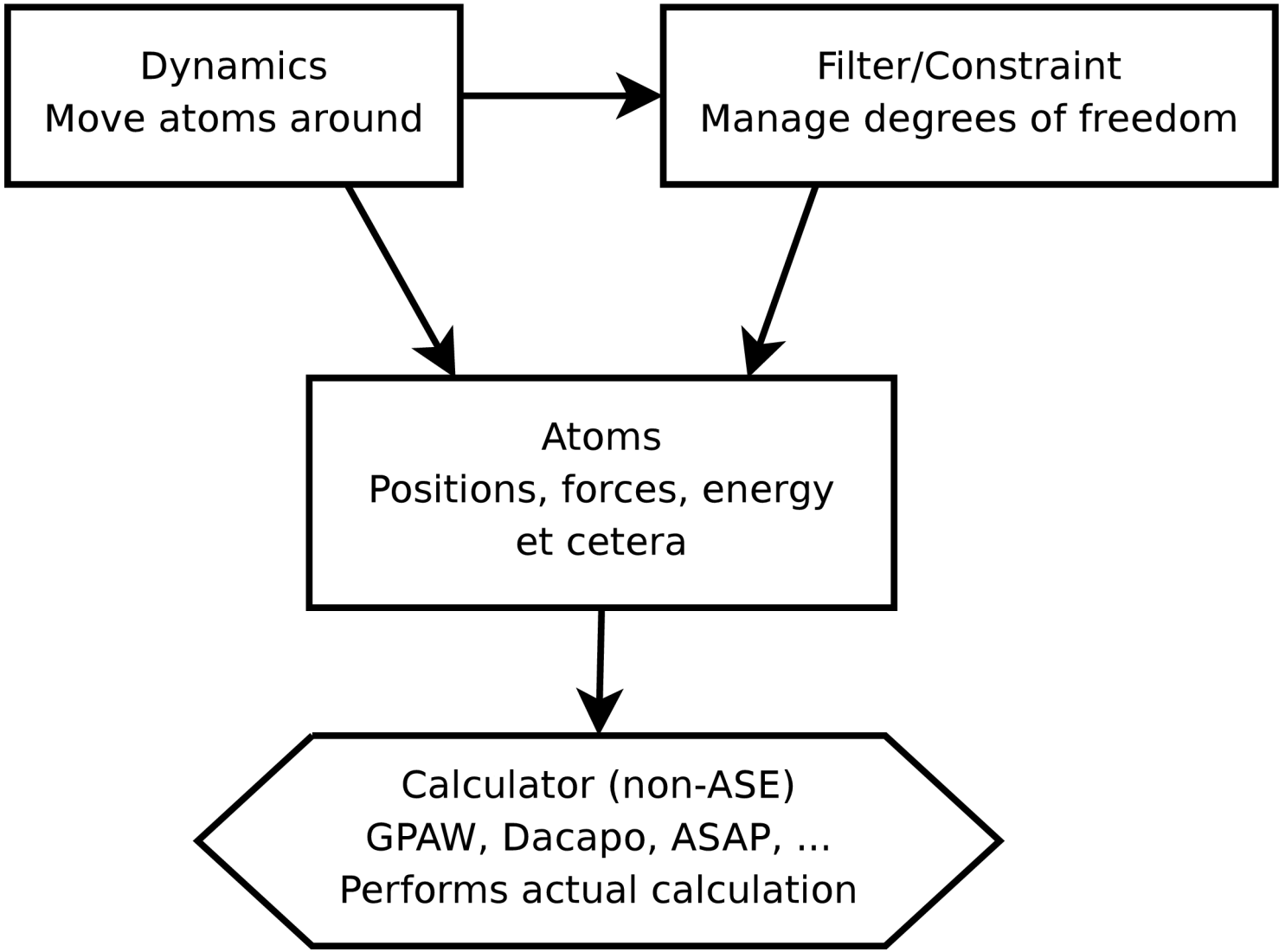
http://www.python.org/

```
from grocery import ingredients
from kitchen import mix, boil

# Start cooking ...
soup = mix(ingredients)

done = False
while not done:
    done = boil(soup)
    print 'boiling ...'

print 'done!'
```

Energy Calculations



ASE Objects


Dynamics
Move atoms around
Filter/Constraint
Manage degrees of freedom
Atoms
Positions, forces, energy
et cetera
Calculator (non-ASE)
GPAW, Dacapo, ASAP, ...
Performs actual calculation

Demonstration

Atomization energy of a H_2 molecule

atomize.py - emacs@neumann.fysik.dtu.dk (på neumann.fysik.dtu.dk)

File Edit Options Buffers Tools IM-Python Python Help

```
from ase import Atoms
from gpaw import GPAW

a = 4.0 # Size of unit cells (Angstroms)
c = a / 2

# Hydrogen atom
atom = Atoms('H', positions=[(c, c, c)], magmoms=[1.0],
             cell=(a, a, a), pbc=False)

# GPAW calculator
calc = GPAW(h=0.2, nbands=1, xc='PBE', txt='H.log')
atom.set_calculator(calc)

e1 = atom.get_potential_energy()
calc.write('H.gpw')

# Hydrogen molecule
d = 0.74 # Experimental bond length
molecule = Atoms('2H', positions=[(c, c, c - d / 2),
                                  (c, c, c + d / 2)],
                 cell=(a, a, a), pbc=False)

calc.set(txt='H2.log')
molecule.set_calculator(calc)
e2 = molecule.get_potential_energy()
calc.write('H2.gpw')

print 'atomic energy:       %5.2f eV' % e1
print 'molecular energy:    %5.2f eV' % e2
print 'atomization energy: %5.2f eV' % (e2 - 2 * e1)
```

--:-- atomize.py (Python)--L32--All----------

```
[askhl@neumann ~]$ python atomize.py
atomic energy:       -0.74 eV
molecular energy:    -6.35 eV
atomization energy: -4.86 eV
```

Script

```
from ase import Atoms
from gpaw import GPAW

a = 4.0 # Size of unit cells (Angstroms)
c = a / 2

# Hydrogen atom
atom = Atoms('H', positions=[(c, c, c)], magmoms=[1.0],
             cell=(a, a, a), pbc=False)

# GPAW calculator
calc = GPAW(h=0.2, nbands=1, xc='PBE', txt='H.log')
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# Hydrogen molecule
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                                  (c, c, c + d / 2)],
                 cell=(a, a, a), pbc=False)

calc.set(txt='H2.log')
molecule.set_calculator(calc)
e2 = molecule.get_potential_energy()
calc.write('H2.gpw')

print 'atomic energy:      %5.2f eV' % e1
print 'molecular energy:   %5.2f eV' % e2
print 'atomization energy: %5.2f eV' % (e2 - 2 * e1)
```
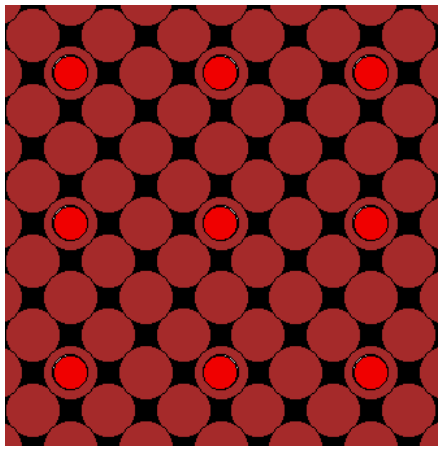
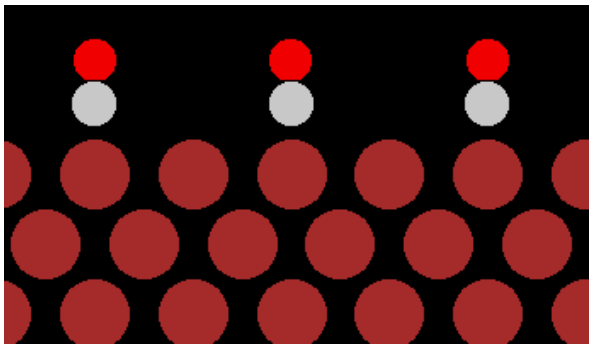

Simple example: CO on Cu(100)

Part II

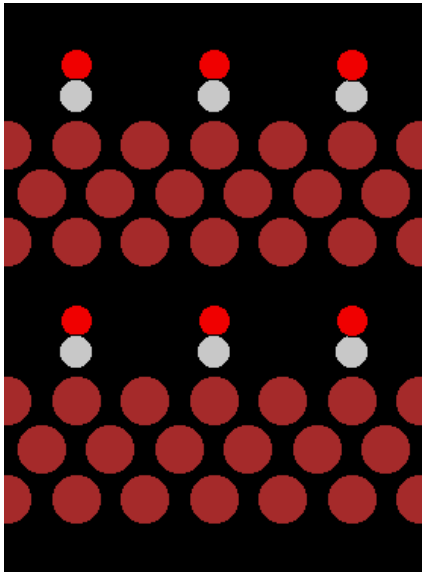
Example: CO/Cu(100)

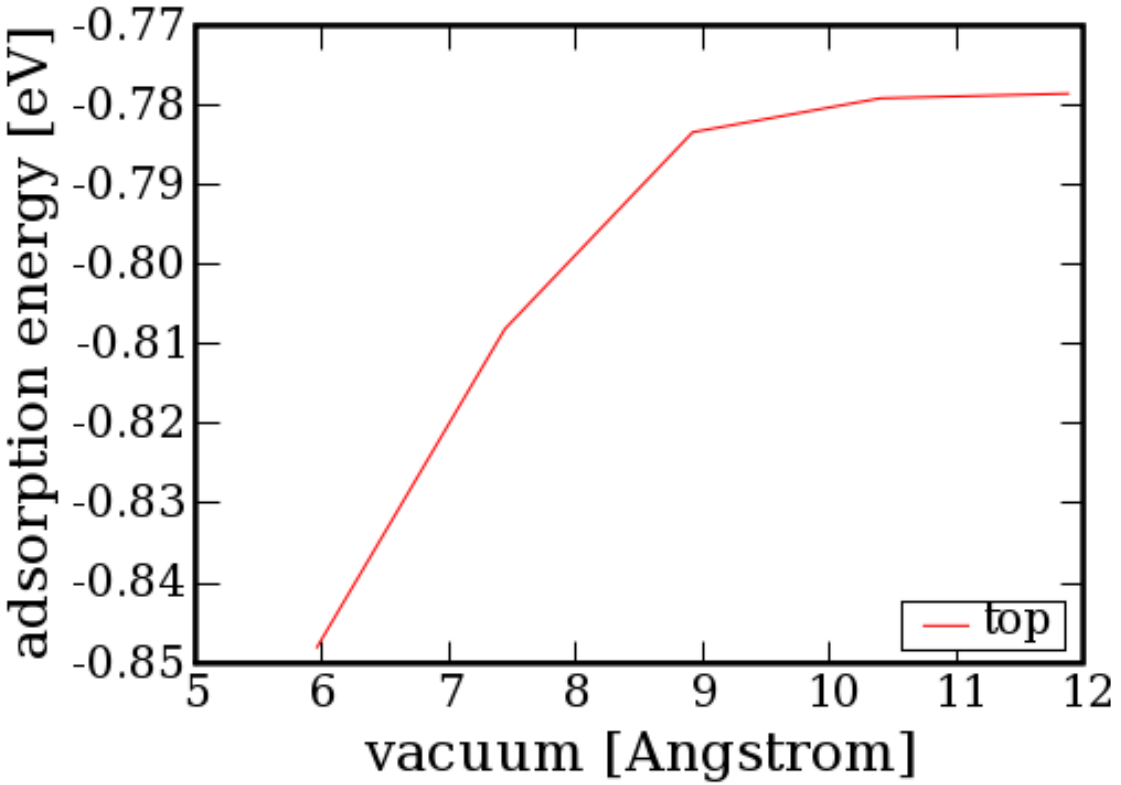
- Calculate adsorption energies for the p(2x2) structure using the PBE functional.
- This will be done by means of a structure relaxation.
  - Calculate forces, move atoms in general direction of forces, repeat until geometry converges.
- Experimental value: 0.53 eV - 0.57 eV

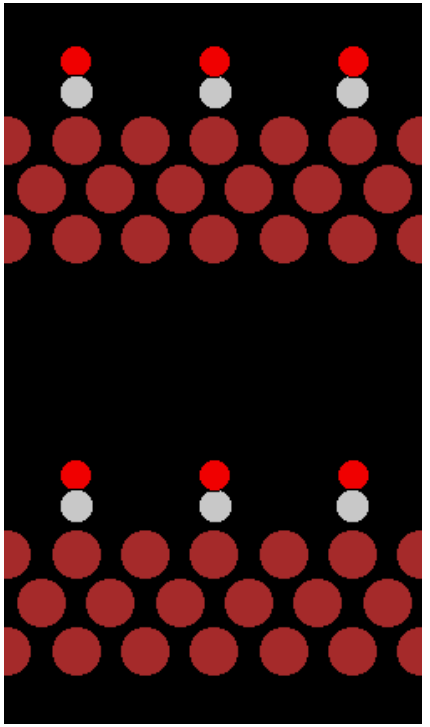




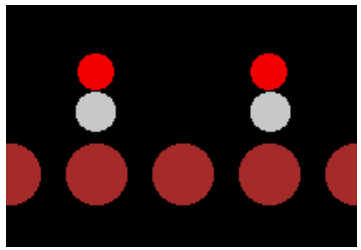
How much vacuum?

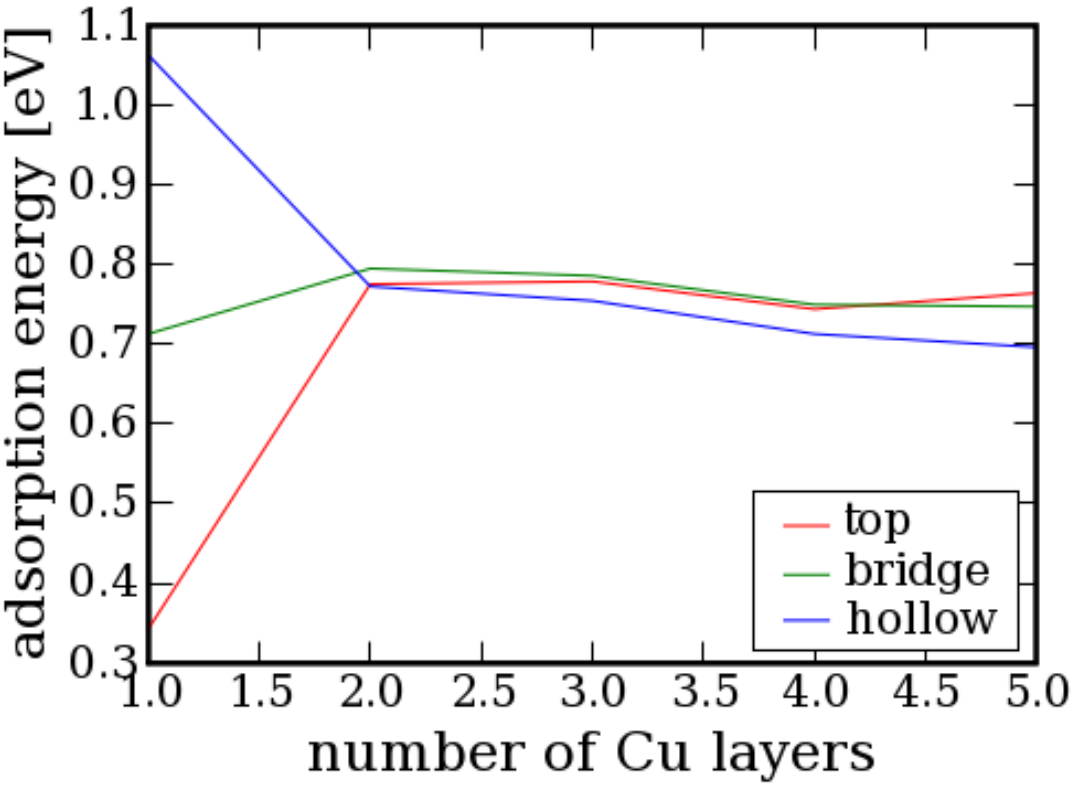


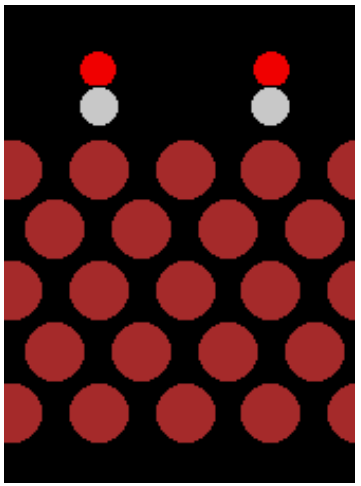




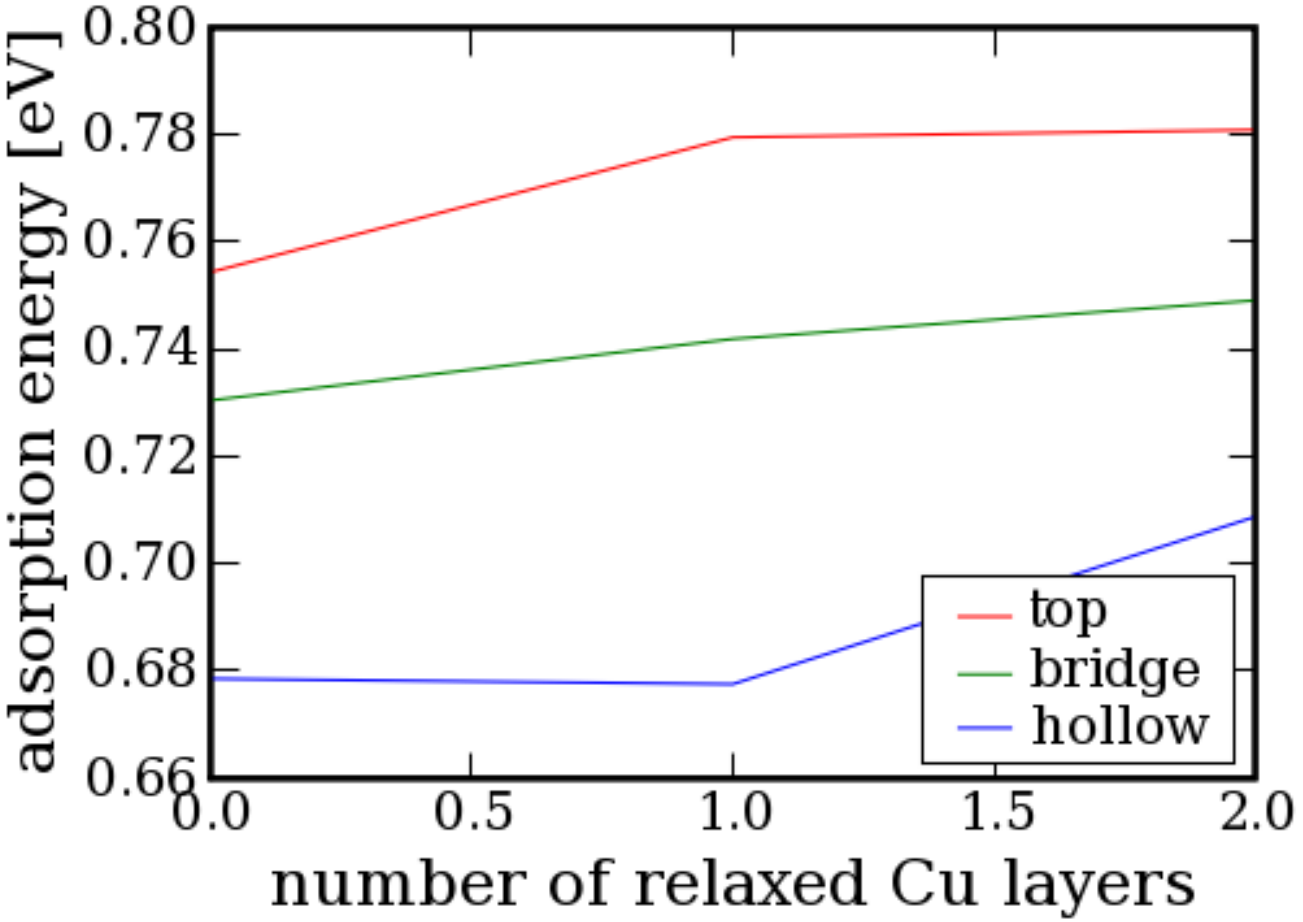
How thick should the slab be?



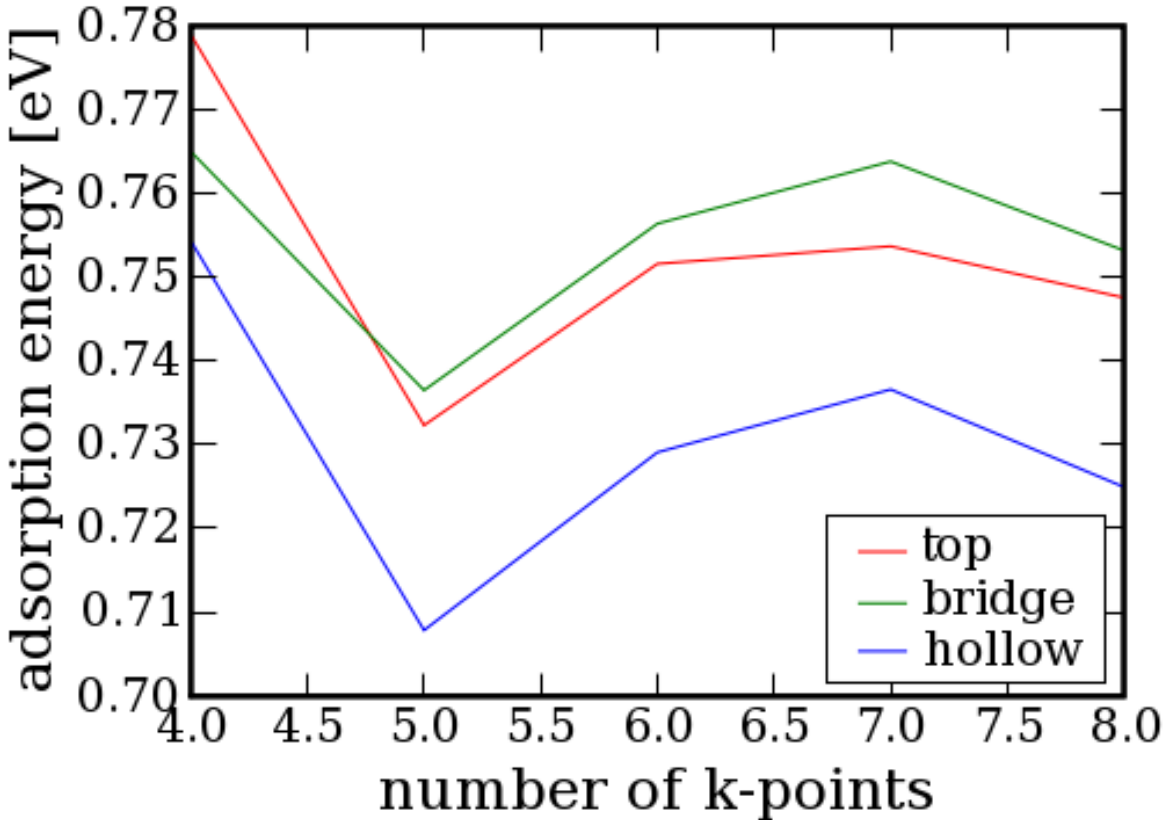




Surface relaxations



Number of **k**-points



- The 2D surface Brillouin zone is sampled uniformly with NxN points.
- GPAW language:
  kpts=(N, N, 1)

Useful Software and Websites

Part III

https://wiki.fysik.dtu.dk

CAMPOS-Wiki

IT-Wiki	Tips and tricks for CAMP computer users
ASE	Atomic simulation environment
Asap	Asap-calculator
Dacapo	Dacapo-calculator
GPAW	Grid-based PAW-calculator
Niflheim	Niflheim Linux supercomputer cluster

- Exercises can be found on GPAW-> Exercises

Software

- Python – The language that ASE uses

http://www.python.org and

- Scientific Python – Addon with nice tools

http://www.scipy.org

- Jmol – Java based molecular viewer

http://jmol.sourceforge.net/download/

- VMD – Multiplatform Visualization tool

http://www.ks.uiuc.edu/Research/vmd/

Software for remote access

- You need a SHELL and X11

- Putty: http://www.chiark.greenend.org.uk/~sgtatham/putty/

- Xming: http://sourceforge.net/projects/xming

- OSX and GNU/Linux run X11 and terminals natively

- Use your Campusnet login to connect to bohr.gbar.dtu.dk

Example:

```
ssh -X s021864@bohr.gbar.dtu.dk
```