# Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

## geometry optimization 3 : atom positions

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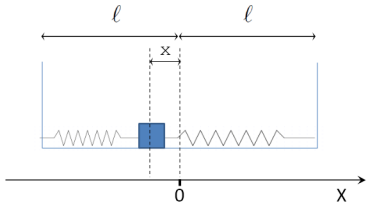
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

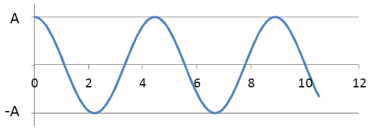
equation of motion in a classical spring problem :

2 identical springs
rest length $\ell$
spring constant k

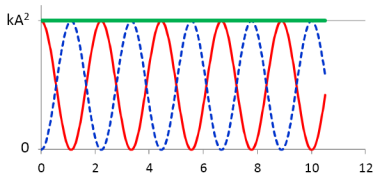



$$\vec{F} = 2k\,\vec{x} \qquad F = -2kx \quad \Rightarrow \quad \frac{d^2x}{dx^2} = -\frac{2k}{m}x$$

time evolution of position when released at t=0 from x=A with no initial speed :

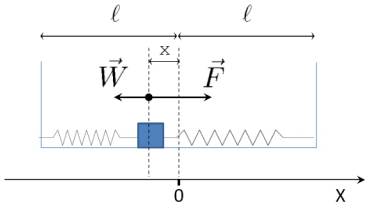


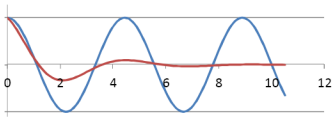

time evolution of kinetic, potential and total energy :



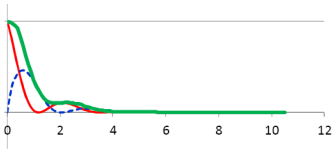

up to infinity...

what happens if there is a friction force that dissipates energy ?




position for undamped and damped oscillator




kinetic

potential

total

energy

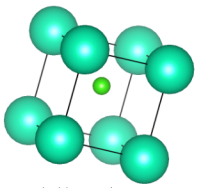
The system comes to rest in a state

- with all forces being zero.
- with no kinetic energy and with potential energy being minimal.

## mimic this with atoms

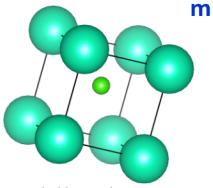
```
data_Wien2k_Data
_cell_length_a    4.122998
_cell_length_b    4.122998
_cell_length_c    4.122998
_cell_angle_alpha   90.000000
_cell_angle_beta    90.000000
_cell_angle_gamma   90.000000
_symmetry_space_group_name_H-M          'P4mm   '
_symmetry_space_group_number   99

loop_
_symmetry_equiv_pos_as_xyz
   +x,+y,+z
   -x,-y,+z
   -y,+x,+z
   +y,-x,+z
   +x,-y,+z
   -x,+y,+z
   -y,-x,+z
   +y,+x,+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Cs001  Cs  0.00000000  0.00000000  0.00000000
Cl002  Cl  0.50000000  0.50000000  0.60000000
```



CsCl with central atom vertically displaced

## mimic this with atoms



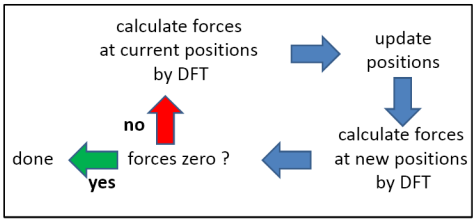
CsCl with central atom vertically displaced

- run a DFT calculation for this cif file, calculate forces (WIEN2k: `run_lapw -cc 0.00001 -fc 0.5`)
- plot forces and total energy as a function of displacement of the Cl atom (WIEN2k: `grep :FGL case.scf` to know forces)

Units : mRy/au (alternative: eV/Å) (SI: J/m , which is N)

straightforward generalization for more than one moving atom in the unit cell : "damped Newtonian dynamics" available in many DFT codes

- give all atoms a fictituous initial speed
- assume a speed-dependent friction force




many subsequent scf cycles

some DFT codes allow for one long scf cycle, where atom positions are continuously changed.

## Concluding exercise

Exercise: $SiO_2$ (stishovite) and $PbO_2$ both have the rutile structure.

ITA 136 ($P4_2/mnm$), Si/Pb=2a, O=4f

- Find or create a cif file
- Do a DFT calculation (`run_lapw -cc 0.0001 -fc 0.1`)
- Save the DFT calculation (`save_lapw -a my-name`)
- Inspect positions and forces (`grep :POS my-name.scf ; grep :FGL my-name.scf`)
- Change the free parameter in the 4f-position
- Calculate and save
- Go on until you have found the positions that make the force zero.
- Plot force vs. position (x) and energy vs. position. What do you observe? Compare to the classical case.