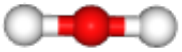
In [2]:
```
from ase.io import read
from ase import Atoms
from ase.optimize import *
from ase.visualize import view
from ase.md import *
from ase.calculators.mopac import *

import nglview
```

In [3]:
```
#
# In this tutoiral notebook, you will optimize a single water molecule
# now using a semi-empirical force-field and the BFGS Quasi-Newton met
#

#
# In 01.01_newton_on_harmonic_potential_of_water.ipynb,
# you saw that from all three starting conformations, the Newton metho
# 1 step because we had used a simple, 2D-harmonic potential for water
# For semi-empirical force fields, however, which also include non-bon
# the "linear" H2O conformation represents a saddle point, on which th
# and not converge to the minimum, whereas a Quasi-Newton method indee
#
# Unfortunately, the Newton optimizer is not implemented in ASE.
# However, we can already sense this saddle-point behavior of the "lin
# using the BFGS Quasi-Newton optimizer and comparing differences in h
# to the minimum structure.
#
# TASK:
# (i)  Optimize the three different water conformations below, with va
#      (e.g. numiterations=2, 5, 10)
# (ii) Comparing the initial and optimized structures through visualiz
#      (via the nglview module below, or VMD, Pymol, ...),
#      can you confirm that the linear water conformation takes longer
#

#model = "h2o"
#model = "h2o_90"
model = "h2o_linear"

# number of optimzation iterations
numiterations = 20

infile  = "input/%s.pdb" % model
water   = read(infile, format="pdb")
molecule = Atoms(water)

# visualize initial structure
wdg_init = nglview.show_ase(molecule)
wdg_init.add_representation('ball+stick')
wdg_init.center_view(range(3))
```

In [4]:
```
# instantiate Mopac
calc = Mopac(restart=0, spin=0, OPT=False, functional='PM6', job_type=

#
# Compare the initial PDB files before and after Optimization - what d
# What is your conclusion with respect to what you know from 01_water_
#

molecule.set_calculator(calc)

print "model", model
ener = molecule.get_potential_energy()
print "potential energy:", ener
grad = molecule.get_forces()
print "gradient", grad

dyn = QuasiNewton(molecule, trajectory = "output/" + model + '.water.Q
dyn.run(fmax=0.005, steps = numiterations)
outfile = "output/" + model + ".QN_opt.pdb"
molecule.write(outfile)
```

```
model h2o_linear
potential energy: -1.40506799782
gradient [[ -3.36939171e-04  -3.22542285e-04   2.85778188e-03]
 [  6.39013593e-04   1.81500502e-03   3.17160516e+00]
 [  6.22626294e-03   4.25974371e-03  -3.15888890e+00]]
BFGSLineSearch:   0[  0]  16:24:36       -1.405068       3.1716
BFGSLineSearch:   1[  1]  16:24:36       -1.995258       1.2994
BFGSLineSearch:   2[  3]  16:24:36       -2.032130       0.0353
BFGSLineSearch:   3[  5]  16:24:37       -2.032146       0.0056
BFGSLineSearch:   4[ 78]  16:24:43       -2.032147       0.0115
BFGSLineSearch:   5[ 87]  16:24:44       -2.134288       1.8143
BFGSLineSearch:   6[ 96]  16:24:44       -2.134299       1.8216
BFGSLineSearch:   7[ 99]  16:24:45       -2.296230       1.2310
BFGSLineSearch:   8[100]  16:24:45       -2.353296       0.2595
BFGSLineSearch:   9[101]  16:24:46       -2.354704       0.0829
BFGSLineSearch:  10[102]  16:24:46       -2.354933       0.0218
BFGSLineSearch:  11[103]  16:24:46       -2.354945       0.0085
BFGSLineSearch:  12[175]  16:24:51       -2.354945       0.0092
BFGSLineSearch:  13[258]  16:24:58       -2.354945       0.0092
BFGSLineSearch:  14[266]  16:24:59       -2.354945       0.0093
BFGSLineSearch:  15[339]  16:25:04       -2.354945       0.0096
BFGSLineSearch:  16[418]  16:25:10       -2.354945       0.0096
BFGSLineSearch:  17[497]  16:25:15       -2.354945       0.0096
BFGSLineSearch:  18[580]  16:25:21       -2.354945       0.0092
BFGSLineSearch:  19[649]  16:25:27       -2.354945       0.0092
```

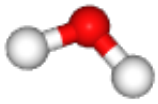
In [5]:
```
# visualize initial structure
wdg_init.display(gui=True)
```



General	Represe	Preferen	Theme	Extra	Help

```
The installed widget Javascript is the wrong version.
The installed widget Javascript is the wrong version.
```

In [6]:
```
# visualize optimized structure
wdg = nglview.show_ase(molecule)
wdg.add_representation('ball+stick')
wdg.center_view(range(3))
wdg.display(gui=True)
```



General	Represe	Preferen	Theme	Extra	Help

```
The installed widget Javascript is the wrong version.
The installed widget Javascript is the wrong version.
```

In [ ]: