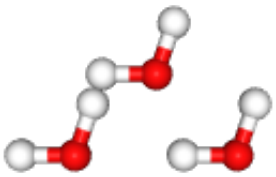
In [1]:
```
from ase.io import read
from ase import Atoms
from ase.optimize import *
from ase.visualize import view
from ase.md import *
from ase.calculators.mopac import *
from ase.constraints import *

import nglview
```

In [2]:
```
#
# In this tutorial notebook, you will explore the physical phenomenon
# for sets of oxygen position-constrained, yet otherwise freely rotata
# For now, consider the set of three such water molecules, whose oxyge
#
instem = "3h2o.flat_triangle"
wdg_init = nglview.show_structure_file("input/%s.pdb" % (instem))
wdg_init.add_representation('ball+stick')
wdg_init.center_view()
wdg_init.display(gui=True)
```



General	Represe	Preferen	Theme	Extra	Help

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

In [3]:
```
#
# optimize the geometry of this water set with BFGS
#

# number of optimization iterations
numsteps = 20
```

```
numsteps = 20

calc = Mopac(restart=0, spin=0, OPT=False, functional='PM6', job_type=

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

# add constraints on oxygen atoms
c = FixAtoms(indices=[atom.index for atom in molecule if atom.symbol =
molecule.set_constraint(c)
molecule.set_calculator(calc)

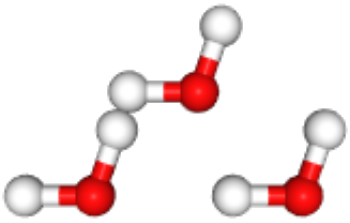
print "model", model
ener = molecule.get_potential_energy()
print "potential energy:", ener
grad = molecule.get_forces()
print "gradient", grad

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

```
model 3h2o.flat_triangle
potential energy: 0.54960155899
gradient [[  0.00000000e+00   0.00000000e+00   0.00000000e+00]
 [ -1.05021277e+00  -9.60058689e-01  -2.60618329e-05]
 [  4.75815783e-01  -1.19315906e+00   9.44904058e-05]
 [  0.00000000e+00   0.00000000e+00   0.00000000e+00]
 [ -1.00337614e+00  -1.43798353e-01   9.05876355e-05]
 [  1.15372348e+01  -2.39985230e+01  -5.07763428e-03]
 [  0.00000000e+00   0.00000000e+00   0.00000000e+00]
 [ -5.60305830e+00   2.60677827e+01  -4.80105795e-03]
 [  2.69996556e-01  -5.55082133e-01   4.79607108e-05]]
BFGSLineSearch:   0[  0]  16:29:07        0.549602      26.6632
BFGSLineSearch:   1[  1]  16:29:08       -4.424703       4.6204
BFGSLineSearch:   2[  2]  16:29:08       -5.205690       3.2730
BFGSLineSearch:   3[  3]  16:29:08       -5.793190       2.9821
BFGSLineSearch:   4[  4]  16:29:09       -6.129457       2.5009
BFGSLineSearch:   5[  5]  16:29:09       -6.335629       0.9288
BFGSLineSearch:   6[  6]  16:29:10       -6.411083       0.6194
BFGSLineSearch:   7[  7]  16:29:10       -6.480944       1.0465
BFGSLineSearch:   8[  8]  16:29:11       -6.519512       0.6799
BFGSLineSearch:   9[  9]  16:29:11       -6.569986       0.6543
BFGSLineSearch:  10[ 10]  16:29:12       -6.605957       0.3437
BFGSLineSearch:  11[ 11]  16:29:12       -6.625449       0.4819
BFGSLineSearch:  12[ 12]  16:29:13       -6.646973       0.3127
BFGSLineSearch:  13[ 14]  16:29:13       -6.660507       0.4100
BFGSLineSearch:  14[ 15]  16:29:14       -6.679270       0.6452
BFGSLineSearch:  15[ 16]  16:29:14       -6.693535       0.3981
BFGSLineSearch:  16[ 17]  16:29:15       -6.714248       0.2238
BFGSLineSearch:  17[ 19]  16:29:15       -6.722937       0.3554
BFGSLineSearch:  18[ 20]  16:29:16       -6.732750       0.3467
```

```
BFGSLineSearch:  19[ 23]  16:29:16       -6.748133       0.4457
```

In [4]:
```
#
# compare the initial structure with ...
#
instem = "3h2o.flat_triangle"
wdg_init = nglview.show_structure_file("input/%s.pdb" % (instem))
wdg_init.add_representation('ball+stick')
wdg_init.center_view()
wdg_init.display(gui=True)
```



General	Represe	Preferen	Theme	Extra	Help

```
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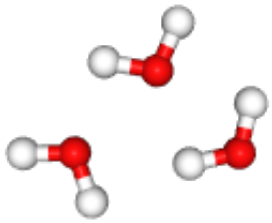
```

In [5]:
```
wdg_final_2h2o = nglview.show_ase(molecule)
wdg_final_2h2o.add_representation('ball+stick')
wdg_final_2h2o.center_view(range(3))
wdg_final_2h2o.display(gui=True)
```



General	Represe	Preferen	Theme	Extra	Help

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

In [6]:
```
#
# Now delete the third water molecule and reoptimize
#

#
# remember optimized structure visualization from above with three H2O
#
wdg_final_3h2o = nglview.show_ase(molecule)
wdg_final_3h2o.add_representation('ball+stick')
wdg_final_3h2o.center_view(range(3))

calc = Mopac(restart=0, spin=0, OPT=False, functional='PM6', job_type=

# delete constraints
del molecule.constraints
# delete third water molecule
del molecule[range(6,9)]

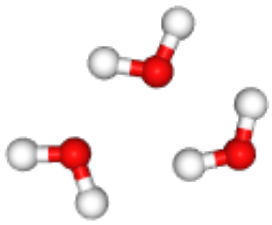
# reintroduce constraints on oxygens
c = FixAtoms(indices=[atom.index for atom in molecule if atom.symbol =
molecule.set_constraint(c)
molecule.set_calculator(calc)
```

```
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 + '.2h2o.QN_
dyn.run(fmax=0.005, steps = numsteps)
outfile = "output/" + model + ".QN_opt.2h2o.pdb"
molecule.write(outfile)
```

```
model 3h2o.flat_triangle
potential energy: -4.74463256631
gradient [[ 0.          0.          0.        ]
 [ 0.15096627  0.48275677 -0.00178664]
 [ 0.38484017  0.11356034 -0.00102339]
 [ 0.          0.          0.        ]
 [ 0.04568566 -0.27464562  0.00126424]
 [ 0.16915179  0.00406309 -0.00147208]]
BFGSLineSearch:   0[  0]  16:30:36       -4.744633       0.5058
BFGSLineSearch:   1[  1]  16:30:37       -4.775554       0.3256
BFGSLineSearch:   2[  3]  16:30:37       -4.790628       0.0894
BFGSLineSearch:   3[  4]  16:30:38       -4.792042       0.0929
BFGSLineSearch:   4[  7]  16:30:38       -4.803314       0.3000
BFGSLineSearch:   5[  9]  16:30:39       -4.816766       0.3480
BFGSLineSearch:   6[ 10]  16:30:39       -4.831528       0.4527
BFGSLineSearch:   7[ 12]  16:30:40       -4.842310       0.2209
BFGSLineSearch:   8[ 13]  16:30:40       -4.844633       0.1104
BFGSLineSearch:   9[ 14]  16:30:40       -4.846993       0.0821
BFGSLineSearch:  10[ 15]  16:30:41       -4.847692       0.0243
BFGSLineSearch:  11[ 16]  16:30:41       -4.847811       0.0180
BFGSLineSearch:  12[ 17]  16:30:42       -4.847869       0.0171
BFGSLineSearch:  13[ 20]  16:30:42       -4.847955       0.0285
BFGSLineSearch:  14[ 22]  16:30:43       -4.848375       0.0779
BFGSLineSearch:  15[ 25]  16:30:43       -4.849837       0.1326
BFGSLineSearch:  16[ 26]  16:30:44       -4.851038       0.1253
BFGSLineSearch:  17[ 27]  16:30:44       -4.852289       0.0544
BFGSLineSearch:  18[ 28]  16:30:45       -4.852745       0.1123
BFGSLineSearch:  19[ 30]  16:30:45       -4.853180       0.0921
```

In [7]:
```
wdg_final_3h2o.display(gui=True)
```



General	Represe	Preferen	Theme	Extra	Help

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

In [8]:
```
wdg_final_2h2o = nglview.show_ase(molecule)
wdg_final_2h2o.add_representation('ball+stick')
wdg_final_2h2o.center_view(range(3))
wdg_final_2h2o.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 [9]:
```
#
# Apparently, the two water molecules alone can adopt a different grou
# their orientation state in G3, with a lower energy.
#
# Reversely, it appears that in the presence of the 3rd water molecule
# are geometrically frustrated, i.e. their orientation from G2 can no
#
# Can you verify this by adding back the third water molecule?
# (
# - copy input/3h2o.flat_triangle.pdb to input/3h2o.flat_triangle.with_
# - in input/3h2o.flat_triangle.with_G2.pdb: replace the coordinates o
#   with the ones from output/3h2o.flat_triangle.QN_opt.2h2o.pdb
# )
```

In [11]:
```
#
# Now add the third water molecule back again and reoptimize
#

calc = Mopac(restart=0, spin=0, OPT=False, functional='PM6', job_type=

model = "3h2o.flat_triangle.with_G2"
water   = read("input/%s.pdb" % (model), format="pdb")
molecule = Atoms(water)
```

```
molecule = Atoms(water)

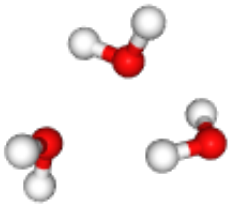
# add constraints on oxygen atoms
c = FixAtoms(indices=[atom.index for atom in molecule if atom.symbol ==
molecule.set_constraint(c)
molecule.set_calculator(calc)

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.QN
dyn.run(fmax=0.005, steps = numsteps)
outfile = "output/" + model + ".QN_opt.pdb"
molecule.write(outfile)
```

```
model 3h2o.flat_triangle.with_G2
potential energy: -6.44853091729
gradient [[ 0.          0.          0.        ]
 [-0.04591327 -0.63339842 -0.07416226]
 [-0.40536605 -0.13406077  0.07204167]
 [ 0.          0.          0.        ]
 [-0.05309376 -0.05881418  0.08077516]
 [ 0.34090807 -0.24020866 -0.17782492]
 [ 0.          0.          0.        ]
 [-1.07741569  1.37254665  0.19757623]
 [ 0.64830175 -0.85336146 -0.02088906]]
BFGSLineSearch:   0[  0]  16:31:06       -6.448531       1.7561
BFGSLineSearch:   1[  2]  16:31:07       -6.585114       0.6310
BFGSLineSearch:   2[  3]  16:31:07       -6.648945       0.3180
BFGSLineSearch:   3[  5]  16:31:08       -6.693037       0.5508
BFGSLineSearch:   4[  6]  16:31:08       -6.730311       0.4207
BFGSLineSearch:   5[  7]  16:31:09       -6.774316       0.2347
BFGSLineSearch:   6[  8]  16:31:09       -6.795461       0.2851
BFGSLineSearch:   7[ 10]  16:31:10       -6.822874       0.4321
BFGSLineSearch:   8[ 13]  16:31:10       -6.882696       0.3963
BFGSLineSearch:   9[ 15]  16:31:11       -6.914559       0.5566
BFGSLineSearch:  10[ 17]  16:31:11       -6.934596       0.3829
BFGSLineSearch:  11[ 18]  16:31:12       -6.958354       0.3531
BFGSLineSearch:  12[ 19]  16:31:12       -6.973277       0.3280
BFGSLineSearch:  13[ 20]  16:31:13       -6.988273       0.4795
BFGSLineSearch:  14[ 21]  16:31:13       -7.005756       0.2284
BFGSLineSearch:  15[ 22]  16:31:14       -7.015619       0.1881
BFGSLineSearch:  16[ 23]  16:31:14       -7.024451       0.2635
BFGSLineSearch:  17[ 24]  16:31:15       -7.031571       0.2230
BFGSLineSearch:  18[ 25]  16:31:15       -7.036474       0.1671
BFGSLineSearch:  19[ 27]  16:31:16       -7.044535       0.1441
```

In [12]:
```
#
# visualize the optimized structure
#
wdg_final_2h2o = nglview.show_ase(molecule)
wdg_final_2h2o.add_representation('ball+stick')
wdg_final_2h2o.center_view(range(3))
wdg_final_2h2o.display(gui=True)
```



General	Represe	Preferen	Theme	Extra	Help

```
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```

In [ ]:
```
# Hä?
# This is very odd:
# After optimization, the water molecules have now orientated out of t

# TASK:
# Can you find an explanatation for what has happend?
```

In [36]:
```
#
# The choice of numsteps = 20 is still too short !
#
# With numsteps = 20, BFGS mostly optimizes the waters' orientations i
# only later does it optimze these orientations in 3D as well.
#
# Check out the input/output files:
# 3h2o.flat_triangle.pdb                          has zero
# 3h2o.flat_triangle.QN_opt.pdb                   has < 0.01 absolute
# 3h2o.flat_triangle.QN_opt.2h2o.pdb              has < 0.03 absolute
# 3h2o.flat_triangle.with_G2.flattened.QN_opt.pdb has significant
#
# very likely, the 2D orientation plane of the three water molecules f
#
```

In [13]:
```
#
# by the way: for numsteps = 20 (not for =100), one can simply set all
# 3h2o.flat_triangle.with_G2.pdb back to zero, and obtain a simular re
# 3h2o.flat_triangle.QN_opt.pdb:

calc = Mopac(restart=0, spin=0, OPT=False, functional='PM6', job_type=

model = "3h2o.flat_triangle.with_G2.flattened"
water   = read("input/%s.pdb" % (model), format="pdb")
molecule = Atoms(water)

# add constraints on oxygen atoms
c = FixAtoms(indices=[atom.index for atom in molecule if atom.symbol ==
molecule.set_constraint(c)
molecule.set_calculator(calc)

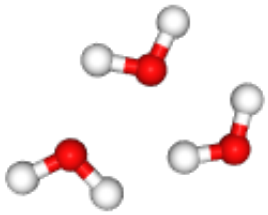
print "model", model
ener = molecule.get_potential_energy()
print "potential energy:", ener
grad = molecule.get_forces()
print "gradient", grad

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

```
model 3h2o.flat_triangle.with_G2.flattened
potential energy: -6.3328445659
gradient [[  0.00000000e+00   0.00000000e+00   0.00000000e+00]
 [  4.23706861e-02  -7.44905292e-01  -4.20198271e-05]
 [ -5.94667065e-01   1.45227547e-01  -6.17071351e-05]
 [  0.00000000e+00   0.00000000e+00   0.00000000e+00]
 [ -3.17650769e-01  -6.78235524e-01  -6.47426232e-05]
 [  1.48405062e+00   1.05653487e+00  -2.24886299e-04]
 [  0.00000000e+00   0.00000000e+00   0.00000000e+00]
 [ -1.21209660e+00   1.49009501e+00  -6.95560399e-05]
 [  6.46041485e-01  -8.48015183e-01   8.70317781e-05]]
```

```
BFGSLineSearch:   0[  0]  16:31:49       -6.332845       1.9208
BFGSLineSearch:   1[  2]  16:31:49       -6.548126       0.6416
BFGSLineSearch:   2[  3]  16:31:50       -6.609120       0.3085
BFGSLineSearch:   3[  4]  16:31:51       -6.636231       0.3255
BFGSLineSearch:   4[  5]  16:31:51       -6.667393       0.2869
BFGSLineSearch:   5[  6]  16:31:52       -6.691684       0.1932
BFGSLineSearch:   6[  7]  16:31:52       -6.702867       0.1504
BFGSLineSearch:   7[  8]  16:31:53       -6.706150       0.2441
BFGSLineSearch:   8[ 10]  16:31:54       -6.712512       0.2248
BFGSLineSearch:   9[ 11]  16:31:54       -6.720436       0.2341
BFGSLineSearch:  10[ 12]  16:31:55       -6.728883       0.2575
BFGSLineSearch:  11[ 14]  16:31:56       -6.740169       0.4311
BFGSLineSearch:  12[ 15]  16:31:56       -6.748813       0.2497
BFGSLineSearch:  13[ 18]  16:31:57       -6.777903       0.4685
BFGSLineSearch:  14[ 19]  16:31:57       -6.793422       0.3484
BFGSLineSearch:  15[ 20]  16:31:58       -6.804015       0.2747
BFGSLineSearch:  16[ 22]  16:31:58       -6.806473       0.1119
BFGSLineSearch:  17[ 23]  16:31:59       -6.811623       0.2675
BFGSLineSearch:  18[ 25]  16:31:59       -6.820068       0.1632
BFGSLineSearch:  19[ 26]  16:32:00       -6.823437       0.1241
```

In [14]:
```
wdg_final_2h2o = nglview.show_ase(molecule)
wdg_final_2h2o.add_representation('ball+stick')
wdg_final_2h2o.center_view(range(3))
wdg_final_2h2o.display(gui=True)
```



General	Represe	Preferen	Theme	Extra	Help

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```

In [ ]: