- When you run the script, you will see some output to the console. This is mostly from the StateData reporter
  - Notice that the potential energy goes slightly up. This is because we started with a minimized structure.
- If you type `ls' again, you will see that the simulation created two files
  - ubq_mod.pdb - the model that includes hydrogen but not water
  - trajectory.dcd - the actual simulation data

```
(openmm) Minh-IIT-MBP2018:[~/Desktop/OpenMM]: python MD_ubq.py
Minimizing...
Running Production...
#"Progress (%)" "Step"  "Time (ps)"     "Potential Energy (kJ/mole)"    "Temperature (K)"       "Speed (ns/day)"
Time Remaining"
10.0%   100     0.20000000000000015     -12936.42476230517      183.51751922475094      0       --
20.0%   200     0.4000000000000003      -12646.180945641867     208.17988992042834      66.3    0:02
30.0%   300     0.6000000000000004      -12391.382319417527     222.92731255729387      63.9    0:01
40.0%   400     0.8000000000000006      -12397.931712869551     252.91336736415292      63.2    0:01
50.0%   500     1.0000000000000007      -12164.42101471391      261.4505010540196       63.7    0:01
60.0%   600     1.2000000000000008      -11959.584803213324     267.99278996281504      63.9    0:01
70.0%   700     1.400000000000001       -11810.354813818332     278.89717139432463      64.1    0:00
80.0%   800     1.6000000000000012      -11819.44354535209      280.87644275577924      64.5    0:00
90.0%   900     1.8000000000000014      -11761.649241585736     281.12817290253514      64.6    0:00
100.0%  1000    2.0000000000000013      -11685.676062540104     281.4727076092732       64.9    0:00
Done!
(openmm) Minh-IIT-MBP2018:[~/Desktop/OpenMM]: ls
1ubq.pdb        MD_ubq.py       trajectory.dcd ubq_mod.pdb
(openmm) Minh-IIT-MBP2018:[~/Desktop/OpenMM]:
```

- To visualize the molecular dynamics trajectory
  - open vmd
  - create a new molecule based on “ubq_mod.pdb”
  - load files “trajectory.dcd” as a file for the new molecule