Exercise 5

Molecular Statistics, Week 5

2014

1 Introduction

Writing simulations is one thing, but sometimes it is also necessary to data-mine, manipulate and visualize data. Python is great for this, and so the goals of this exercise is:

1. Use Python to load/read data
2. Use numpy to manipulate data
3. Use matplotlib/pylab to illustrate
4. Save Numpy data

1.1 Changeing the look of matplotlib

2 Exercises

Which will be done with small individual exercises.

2.1 Dissociation Energy of Water Dimer

distance of the hydrogen bond is defined as the distance between the oxygen and the hydrogen

1. Convert the distance from A.U. to Ångstroem.
2. Convert the energy to kJoule/mol. Plot the result
3. Convert the energy to kcal/mol. Plot the result.

2.2 Proton transfer / reaction path

2.3 Lars Fitting

2.4 some kind of 3d plot