Overview CHEM3011 Comp Skills Resources

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Pre-existing resources
Pre/post-lab resources
Resources to write

1 Comp Skills 1: Building structures IQMol

1.1 Understanding IQMol GUI

Introduction to IQmol.pptx

1.2 Imposing symmetry

(This is already covered briefly in Introduction to IQMol)

1.3 Calculating Electrostatic Potentials (ESP)

How to calculate ESPs, partial charges, and should you believe them?.pdf (IQMol Intro II has a brief set of instructions about NBO. Want to make figures

1.4 Molecular Orbitals

(Introduction to IQMol does a few of these, if you want more see below)
http://www.q-chem.com/Teaching%20Materials/QChemCompLabs/Lab2-MOLCAO.pdf

2 Comp Skills 2: Calculating Chemical properties

2.1 Minimisation and molecular mechanics

A note on molecular mechanics.pdf

2.2 Exploring minimum energy structures

https://www.q-chem.com/Teaching%20Materials/QChemCompLabs/Lab1-IQmol-Intro.pdf (Needs some context, too much asssumed knowlodge)

2.3 Reactions and S_N2 transition states

http://www.q-chem.com/Teaching%20Materials/QChemCompLabs/Lab-Reactions.pdf
(this is pretty good and shows the application)

2.4 Solving harder problems (optional - maybe cut?)

Computational Chemistry Challenge Sets.pdf (open-ended submission)

3 Comp Skills 3: Working with python, Jupyter-notebooks, and matplotlib

3.1 Getting started with Jupyter Notebook

Server details and log in.pdf
What is Jupyter Notebook for and how do you use it?.pdf

3.2 Analysing and plotting complex data

Getting started with plotting.ipynb
Functions and list manipulation for graphing.ipynb
Plotting chemical problems.ipynb

- Speciation Plots
- Hammet Plots (or something else chemical to analyse)

3.3 Exercises for them to complete code/plots for themselves

Small open challenges with automarking feedback.ipynb
(see if nbgrader and plotchecker will work)

4 Comp Skills 4: Representing Complex Data

4.1 Reading data from a spreadsheet/.csv file

either numpy.getfromtxt() or pandas (maybe just mention that pandas is a more powerful solution but would take time to learn)

4.2 PES: 3d plots and contour surfaces

- Example PES of something like H2 + H, show TS saddlepoint
- classic reaction diagram, but point out this needs a choice of 'reaction coordinate'

- 3d plot juxtaposed with contour plot
- Give them external spreadsheet file to read energies from
- get them to pick the right reaction coordinates to plot, and they can just stick in those array variable
- a more general exposition and exploration on why PESes and important

4.3 Transformations of raw data

- Something they need to transform, don't nessecarily tell them how
- Get them to write very simple functions and apply them in a for loop to all data points
- Give them exercises with raw experimental data and they need to come up with a good plot, these can be manually graded (maybe give them time to hand in after class)