Homework 1 - Due 9/6/2012

John Kitchin

2012-09-01 Sat

Instructions: All calculations should be performed in python. You should turn in the code used, and the answers you got.

1 Signup for an account at gitHub.

Print your username here:

Set yourself up to watch https://github.com/jkitchin/dft-course and https://github.com/jkitchin/dft-book.

2 Read Chapter 1 in the text book.

3 Read Section 4 in dft-book.

As part of this assignment, please turn in a pdf copy of dft-book that has been annotated by sticky notes using Adobe Acrobat Reader (you should be able to type Ctrl-6 to get a sticky note while the pdf is open, and then you can move it where you want and type text in it.). Please note any typos, places that are confusing, etc...

4 Data fitting.

Fit a cubic polynomial to this set of data and estimate the lattice constant that minimizes the total energy. Prepare a figure that shows the data, your fit and your estimated minimum. Hints: `numpy.polyfit`, `numpy.polyder`, `numpy.roots`, `numpy.linspace`, `numpy.polyval` will all help you do this easily.

lattice constant ($\mathring{A}$)	Total Energy (eV)
3.5	-3.649238
3.55	-3.696204
3.6	-3.719946
3.65	-3.723951
3.7	-3.711284
3.75	-3.68426

5 Nonlinear algebra

Solve this equation: $\sin(x^2) = 0.5$ for x. Prepare a plot of the function and show where your solution is. Hint: `scipy.optimize.fsolve`

6 Linear algebra

Solve these equations using python and linear algebra:

$$a0 - 3a1 + 9a2 - 27a3 = -2 \quad (1)$$
$$a0 - a1 + a2 - a3 = 2 \quad (2)$$
$$a0 + a1 + a2 + a3 = 5 \quad (3)$$
$$a0 + 2a1 + 4a2 + 8a3 = 1 \quad (4)$$

Use linear algebra to verify your solution. Hint: see `numpy.linalg`, `numpy.dot`.