Data Processing with MATLAB—An Activity

This will be your first interaction with a regular MATLAB script. First copy all three files from the class folder to your personal MATLAB drive. Then make sure the three files ‘TiO.m’, ‘parseXML.m’ and ‘formationenergy.xml’ are in your active path (showing under the right hand side window “Current Folder”).

Look at each of the files. TiO.m is the main MATLAB script you will run, parseXML.m contains MATLAB functions, and formationenergy.xml is a tagged data file containing formation energies and various other parameters for a range of titanium and oxygen containing species.

Formationenergy.xml

Reads Data

parseXML.m

Calls Function

TiO.m

Run the script by typing TiO in the command window. Note the output in the command line and the figures that are generated. You can also investigate the data structures by double clicking on the values in the “Workspace” window. The variable “all\_data” contains the data from the xml format.

Questions:

1. Determine composition of lowest and highest energy materials. There are multiple ways to do this but the min and max functions may be useful (check help menu). Ideally, you should be able to modify the code to print out the information you are looking for here. Comment on what it means for an ionic compound to have a lower formation energy.

Composition of lowest energy material:

Composition of highest energy material:

1. Generate a plot of energies based on the number of titanium atoms (similar to the one for oxygen atoms that is already generated). Comment here on similarities and differences between the energies vs. number of Ti atoms and energies vs. number of O atoms. Save your plot as a jpeg image file with the file name TiAtoms\_*LastnameFirstname*.jpg (your last/first name of course!) and upload this image to the course drive.
2. Explain why one of the points with 2 oxygen atoms is at a significantly higher energy than the others.
3. Explain what is stored in the vector array tio2\_energies and give another way the average TiO2 energy could be determined using this vector.
4. Compute the average energy for all compounds with the empirical formula TiO3. What can you say about the stability of these compounds relative to those with formula TiO2.

Average energy of compounds with empirical formula TiO3:

1. Compute the standard deviation, σ, for TiO2 and TiO3 compounds using the function std(). What does it mean to have a larger standard deviation?

Standard deviation of TiO2 compounds:

Standard deviation of TiO3 compounds:

Harder Questions

1. To determine if the average energy of TiO3 is significantly different from the average energy for the TiO2 compounds, a statistical *t*-test for a difference in means can be performed. To do this in MATLAB, use the function ttest2, use the help menu to make sure that you are not assuming the variance (standard deviation squared) in both samples is equal. The *t*-test returns a value of 1 if the means are different (within 5% error by default) and 0 if the means are identical. Using the *t*-test, are the difference in formation energies for TiO2 and TiO3 significantly different? What is the probability that they are the same?
2. Extract the volume of the unit cell and plot the energy vs. volume. You will need to dig into the data structure to fine where the volume is stored. Save this plot as a jpg figure. Is there a correlation between the energy and the size of the unit cell? Justify your answer.
3. What other quantities or correlations could be interesting to compare? Consult the data available in the xml structure as you think about this question.