

Spreadsheet Applications for Materials Science

Suggestions and Hints for Building Your Spreadsheets

Spreadsheet programming has a lot in common with programming languages such as FORTRAN, Pascal and C, such as defining variables, using functions, handling large blocks of data at one time, and devising numerical techniques for cases where analytical solutions are not available. It also includes practices and conventions that help prevent writing “spaghetti code”, unmanageable, unreadable programs that even the author has trouble understanding. Spreadsheet programming also has a lot in common with documents such as laboratory reports in that the procedure and the results must be easy to read and understand. This document offers practical advice for building your spreadsheet, such as using functions, creating graphs and numerical techniques, plus writing a spreadsheet that is easy to understand, read.

Example

The figure at the end of this document provides an example of how relatively simple calculations can be handled using a spreadsheet. This spreadsheet is easy to read and it is easy to see how the calculations were performed. Because it was built in sections it was also easier to write and debug and it all fits onto a two-page printout. Note that it would be very easy to modify this spreadsheet to handle these calculations for any number of ionic compounds.

Layout

Readability Your spreadsheet should be easy to read and interpret by another person. It should have a header that includes your name, date, title and description of the spreadsheet, etc. The actual calculations, figures and all parameters should be organized and presented in a logical manner.

Organization Organization is the key to being able to quickly build this spreadsheet and, eventually, extending its usefulness. Keep input and other key parameters separate from the main calculations and use a series of tables that handle each part of the assignment. Design these tables so that the information in each is easily accessible in other tables.

Appearance Appearance counts. If the results are useful then the spreadsheet is likely to be shown to and shared with others, revisited in the future, and expanded. Appearance, including overall organization, labels, etc. all count when it comes to presenting your work to others and when maintaining the project.

Typos Minor errors hint of the existence of more serious errors. Even minor spelling and formatting errors in labels and text, which to the author may be merely cosmetic defects, to another person may plant seeds of doubt. After all, simple typos in the formulas are just as easy to make but can be more difficult to detect.

Calculations

Define Define all parameters before using them. Do not enter values, except constants which never change, such as the 2 in $d=2\pi$, in the formulas as this severely limits the usability of your spreadsheet.

- Precision Keep in mind that the precision displayed in a cell may not show its full precision. For example, π may be displayed as 3.14, but greater precision may be needed in your calculations. (In the case of π your spreadsheet has a π function: pi() in Excel, @pi in Quattro Pro. If it doesn't, the formula 4 tan(1) will work just as well.) Using full precision in π , physical constants, conversion factors, and any other critical constants is highly recommended.
- Simplify Break up complex calculations into smaller, more manageable parts. For example, do the calculation in parts using a series of cells, columns or tables instead of entering a single complicated formula in one cell, column or table.
- Simplify Break up larger projects into smaller, more manageable parts. Use separate sheets in a notebook for different stages of the project. Each sheet can then be read, studied, analyzed, and even printed separately.

Analyses

- Trend Line A trend line can be used to plot a line through your data and to quickly determination of the slope and intercept for the data in a graph. Note, however, that these values will be truncated and may lead to errors in subsequent calculations. If this appears to be the case, use the regression procedure instead of or in addition to the trend line.
- Solver Use the solver to find the solution to formulas for cases where only one variable is changed. Solver will find a value in the input cell that will produce the desired result in a formula cell. Both the target error and the maximum number of iterations can be specified.
- Optimizer Use the optimizer to find the solution to a formula for the case where more than one variable is involved. Optimizer requires a variable cell or block of cells, a solution cell and will find the values of all variables that will produce the specified result. This result could be a maximum, minimum or a specified value. Constraints can be placed on the variable cells.

Graphs and Charts

- Titles Do not use the standard titles and subtitles for graphs that will be used in your report. Instead, use figure captions like those used in your text book.
- Frame Color Do not use the default gray color that many spreadsheets use in their graphs. A gray background can be useful if data is plotted using light colors such as yellow, but a white background, like those in your text books, is preferred. Obviously, this also means that you won't want to use yellow or other light colors for the lines and data points.
- Color Color can be used to make your graphs look more attractive, interesting and to help differentiate between sets of data. The use of color, however, must be thought through. For example, consider your final output device. Unless your laser printer or photocopier supports color then it may be better to avoid using color and instead use different line styles.

2nd Y Axis Using a second y axis can allow one to combine different types of data, for example, strength and ductility, into one graph. This can save you and your reader work, will save space in your report, and can be a very effective way to illustrate their relationships to the same independent variable.

Log Scaling Most spreadsheets support log scaling. Usually log scaling will also force you to go with its automatic scaling routines. If automatic scaling is not giving the results you need then it might be better to calculate the log of your data and use linear scaling.

Printing

Range It is not always necessary to print out the whole spreadsheet. Some spreadsheets, after all, use several thousand rows and many more columns than can be shown on one page. It may be sufficient to print the header section of your spreadsheet, or you might want to create a summary page that contains the most important information. Another alternative, design your spreadsheet so that the information that must be printed is all in one area and that area will fit easily into a one or two page printout.

Scaling Printouts can be scaled so that even very large spreadsheets can be printed on one page. (You might even be able to read it if you use a good printer and a microscope.) Use the print scaling capability of your spreadsheet to fit the region of interest onto the number of pages allotted. The printout for the spreadsheet shown in figure 1 was scaled to print one page wide and 2 pages long.

Page Breaks If your printout splits tables of figures at inconvenient places you can insert page breaks just before the table or figure. The horizontal line in figure 1 is a page break that forces the spreadsheet to print the graphs on the second page.

Other

Strings You can combine string (text) data from different cells by concatenating them. For example, you might want to combine the solute and solvent into one string that can be displayed on your charts. To do this enter A1&"'"@A2 to combine the contents of cell A1, which contains "Cu", and cell A2, which contains "Zn", to obtain the string "Cu/Zn".

Frequent Saves

Save your work often. Computers are clearly more reliable these days but, things happen. Quattro Pro and many other applications offer timed backup procedures and these have saved many people's work. Use this feature. (For Quattro Pro type *ALT+F12* and check file options settings. For Excel look for the AutoSave item in the tools menu. If it is not there load the AutoSave addin.) In addition, save your work often, manually. This can be as simple and quick as typing *ALT+F+S* or *CTRL+S* every so often, for instance, after completing a segment of your work.

Keyboard Shortcuts

Keyboard shortcuts can be very useful. It is often easier, when already typing data and formulas, to type the shortcut instead of picking up the mouse over and over again.

Add-ins Microsoft Excel uses an “add-in” feature so that you can load only the specialized features you need. You will probably need the AutoSave, Solver, and Analysis Toolpack for your spreadsheet projects.

Revisions Don't forget to change the revision date whenever you modify the spreadsheet.

Quattro Pro 10 - [C:\Documents and Settings\Adminis...\Sample Spreadsheet.qpw (unmodified)]

File Edit View Insert Format Tools Window Help

Practice:A41 Reference Lattice Energy:

1	File:	Preparation for the Ionic Bonding Experiment.qpw			
2	Owner:	Mike Meier			
3	Created:	January 4, 2003			
4	Revised:	March 21, 2003			
5	Description:	Practice calculations of ionic bonding energies, equilibrium spacing and density of NaCl-type compounds.			
6					
7	Conversion Factors				
8	To convert from	To	Multiply by		
9	Joules	eV	6.242E+18		
10					
11	Physical Constants				
12	Avogadro's Number:	6.022E+23	per mole		
13	Proton Charge:	1.602E-19	C		
14	Permittivity:	8.854E-12	C ² /Nm ²		
15					
16	Material Parameters				
17	Substance:	KCl	RbF	LiI	
18	Mineral Name:	Sylvite	-	-	
19	Lattice Parameter:	0.629170	0.565160	0.600000	nm
20	Coordination Number:	6	6	6	
21	Number of Cations:	4	4	4	per unit cell
22	Number of Anions:	4	4	4	per unit cell
23	Valence of Cation:	1	1	1	
24	Valence of Anion:	-1	-1	-1	
25	Atomic Weight of Cation:	39.0983	85.4678	6.941	g/mole
26	Atomic Weight of Anion:	35.453	18.9984032	126.90447	g/mole
27	Madelung Constant:	1.747565	1.747565	1.747565	
28	Repulsive Energy Parameter:	2132.5	1851.6	623.1	eV
29	Repulsive Range Parameter:	0.0326	0.0301	0.0366	nm
30	Reference Lattice Energy:	-7.190	-7.866	-7.706	eV
31	Reference Density:	1.988	3.844	4.116	Mg/m ³
32					
33	Calculations				
34	Equilibrium Spacing:	0.3146	0.2826	0.3000	m
35	Equilibrium Lattice Energy:	-1.149E-18	-1.275E-18	-1.180E-18	Joules
36	Mass of Unit Cell:	4.952E-22	6.939E-22	8.890E-22	g/unit cell
37	Volume of Unit Cell:	0.2491	0.1805	0.2160	nm ³
38	Density:	1.988E-21	3.844E-21	4.116E-21	g/nm ³
39					
40	Results				
41	Reference Lattice Energy:	-7.190	-7.866	-7.706	eV
42	Calculated Lattice Energy:	-7.171	-7.957	-7.365	eV
43	Difference:	-0.27%	1.16%	-4.42%	
44					
45	Reference Density:	1.988	3.844	4.116	Mg/m ³
46	Calculated Density:	1.988	3.844	4.116	Mg/m ³
47	Difference:	0.01%	-0.00%	-0.00%	
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Header Section

Constants

Variables

Calculations

Results

Graphs and Illustrations

Figure 1. Differences in measured and calculated lattice energies.

Figure 2. Differences in measured and calculated densities.

Figure 1 Montage of three screen shots of a single spreadsheet that calculates the lattice energy and density of three ionic compounds. This spreadsheet was built in sections and can easily be modified to preform these calculations for more than three compounds and for other properties.