# *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 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 parameter 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 — Just like other written work, appearance counts. Aesthetic issues aside, a tidy, organized, and annotated spreadsheet makes them easier to read and therefore more effective. It also tells the reader that extra thought and care was taken in the doing work. Things to consider are spelling and grammar, numeric format, highlighting and color, borders in tables, etc.

***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".

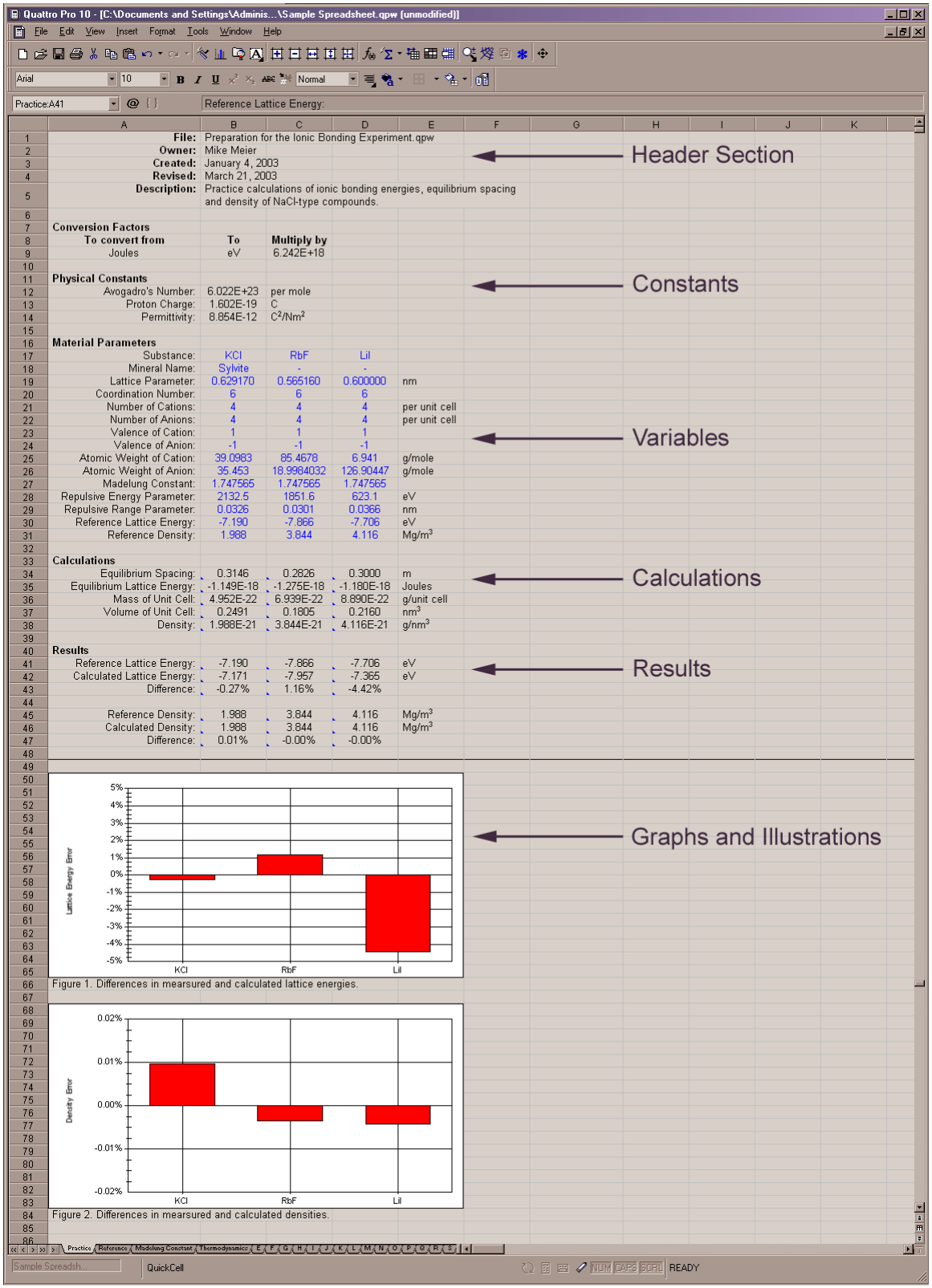


**Figure 1** Montage of three screen shots of a single spreadsheet that calculates the lattice energy and density of three ionic compounds. This spreadsheet was built in sections and can easily be modified to preform these calculations for more than three compounds and for other properties.