[A] Research the primary features of an important chemical/material class of crystal structures. Give a 5-minute PowerPoint presentation at the beginning of the next class period on your findings. The points of interest to discuss will depend to some extent on the classification that you choose. Topics that might be interesting include bonding, bond lengths, atomic close packing, coordination, intermolecular interactions packing, typical symmetries, variable stoichiometry, network connectivity, interstitial sites, crystal appearance (size, color, habit), chirality, density, material properties, material functions or applications.

[B] Become familiar with a computational algebra software package like Maple, Matlab, MathCAD or Mathematica. I prefer Mathematica 6.0 and encourage you to get it installed on a computer that is readily available within your research group. To become familiar with Mathematica, you can download and work through the first four sections Lab 14 from my Physics 230 course (http://www.physics.byu.edu/faculty/campbell/physics230). This notebook (.nb) file contains an introduction to the most basic features of Mathematica. Be sure to include a screen shot at the end of your PowerPoint presentation, from the algebra software of your choice, showing simple examples of $3 \times 3$ matrix multiplication, matrix inversion, and the calculation of a matrix determinant.

[C] Use ISODISPLACE (http://stokes.byu.edu/isodisplace.html) to build, save, upload, and visualize the following three cubic structures. Include a screen shot of one of your structures at the end of your PowerPoint presentation (do a screen grab, e.g. print screen to obtain graphic).

Diamond: space group 227 ($Fd-3m$), $a = 3.56$ Å, one unique C atom at the $a(1/8,1/8,1/8)$ site. When prompted, switch from default origin-choice #2 to origin-choice #1 to get a better view.

SrTiO$_3$ perovskite: space group 221 ($Pm-3m$), $a = 4.2$ Å, three unique atoms: Ti at $a(0,0,0)$, Sr at $b(1/2,1/2,1/2)$ and O at $d(1/2,0,0)$.

Zeolite faujasite: space group 227 ($Fd-3m$), $a = 25$ Å, one unique Si at $i(-0.054, 0.121, 0.0364)$. We don't include the three unique oxygens.

[D] Obtain access to the Crystal Maker software (arrange this with your instructor). Browse the hard drive for the Crystal Maker crystal-structure library, and visually explore a variety of different types of crystal-structures. Please be careful not to save any of your modifications to library structures!!! Browse to Minerals $\rightarrow$ Non-silicates $\rightarrow$ Oxides $\rightarrow$ Perovskite Group $\rightarrow$ BaTiO$_3$. In the main menu, select Transform: Set Range and adjust the range values to display different portions of the crystal. Explore each of the options available in the Model menu. Select the Edit: Structure menu option to see the structural details. Use the Edit: Bonds menu option to modify which interatomic bonds are shown. Try the cursor tools in the Tools palette (visible whenever you have a structure open) to do things like measuring bond lengths and angles. Include one really nice screen shot in your PPT presentation.
[E] Crystal families and lattices
(1) Illustrate and label each of the 5 two-dimensional lattice types.
(2) Draw a centered 2D oblique lattice. Why isn't this listed as one of the 5 standard 2D lattices?
(3) Name the six three-dimensional crystal systems and describe their cell parameters.
(4) In your own words, name and describe each of the 14 three-dimensional Bravais lattices, including centering vectors that they might have.
(5) A face-centered tetragonal cell is equivalent to one of the 14 standard Bravais lattices. Which one is it? Why don't we list this lattice type as face-centered tetragonal instead.
(6) Give an alternate description for a base-centered orthorhombic lattice.

[F] Equivalent unit cells for a given lattice
For any given unit cell, there are infinitely many equivalent cells, but only one unique reduced cell. The reduced cell is the one with the three shortest non-coplanar edges, such that \( a \leq b \leq c \), and all angles are either less than 90° or all angles are greater than 90°. In two dimensional lattices, one merely needs the two shortest non-colinear edges such that \( a \leq b \).
(1) On the square 2D lattice on the next page, use a pencil to highlight five unit cells of area = 1, each of which have a different shape (not merely a different orientation). The cells do not need to include the origin point; they only need to fit within the frame. Show a determinant calculation for each cell to verify its area. Next, use a colored pen to highlight the reduced cell.
(2) Repeat the previous exercise for the oblique 2D lattice on the same page, but without any determinant calculations. You may check your work using the Mathematica-generated cell-viewing tools provide in class, but ONLY after you have completed the exercise.

[G] Relationships between the cell parameters, the lattice basis, and the cell volume
Consider the triclinic unit cell \((a = 3, b = 4, c = 5, \alpha = 60^\circ, \beta = 90^\circ, \gamma = 105^\circ)\). You may use a package like Mathematica to do the following computations; but you must at least show your work in the form of printed input and output.
(1) Write a routine called \texttt{dcell2dbasis} that takes a set of direct-space cell parameters as input and returns a standard \( B \) matrix as output. Demonstrate this routine on the triclinic cell parameters provided.
(2) Compute a triple product of basis vectors to obtain the volume of the unit cell.
(3) Compute the determinant of the \( B \) matrix to obtain the volume of the unit cell.
(4) Write a routine called \texttt{basis2cell} that uses dot products and the cosine rule on the columns of a \( B \) matrix to recover the unit cell parameters. Demonstrate it on the \( B \)-matrix obtained above.

[H] The relationship between the direct-lattice and reciprocal-lattice bases
(1) Write a routine called \texttt{basis2basis} that takes a set of direct-basis vectors (in the form of a \( B \) matrix), and returns the corresponding reciprocal-lattice basis vectors (in the form of a \( B^* \) matrix). This should be a very simple task (matrix inverse transpose). Demonstrate your routine on the triclinic basis from the previous exercise.
(2) Demonstrate that \texttt{dcell2dbasis}, \texttt{basis2basis}, and \texttt{basis2cell}, when used in sequence, are able to convert direct-lattice cell parameters into reciprocal-lattice cell parameters. Use the triclinic cell above as an example. Also show that the same three operations on the reciprocal-lattice cell parameters recovers the original direct-space cell parameters.
(3) Create a simple set of cell parameters for each of the following crystal families (monoclinic, orthorhombic, cubic, trigonal and hexagonal, and determine the corresponding reciprocal-space cell parameters for each one.