Chemical bond analysis

1. Types of chemical bond in molecules

1.1. Visualize the ELF files for ethane, ethylene (ethene), ethyne, choloro-ethane and ethanol molecule. How is the C-C bond evolving? Visualize the lone pairs for ethanol and chloro-ethane molecules. Can you explain the differences? Does this conform to Lewis theory?

1.2. Use TopMod to calculate populations. Can you explain the differences? Does this conform to Lewis theory?

1.3. Visualize the NCI files for water dimer and benzene dimer. Compare the interactions found.

2. Types of chemical bond in solids.

2.1. Use ELF and NCI files for NaCl, diamond, CO_2 and Na to classify the chemical bond present in these solids. Comment on the results.

2.2. Calculate the CHGCAR and the ELFCAR of Na at high pressure. Use it to visualize ELF and NCI. What do you see?

3. Analysis of phase transitions and chemical change.

The hexagonal polymorph of diamond (lonsdalite) belongs to the $P6_3/mmc$ group with $c/a = (8/3)^{1/2}$ and $u = 1/16$. This ideal structure has the same nearest-neighbor environment for each atom as diamond. When $u = 0$ this structure becomes a set of graphitic sheets. Thus, this group can be used to easily mimic the graphite-diamond transformation.

3.1. Using the Bilbao crystallographic server (http://www.cryst.ehu.es/) find a transition path from buckled graphite ($P6_3mc$) to hexagonal diamond (lonsdalite).

3.2. The Cmcm geometry has been used to produce the .cube files provided in the repository. Observe and comment the changes in chemical bond that take place along the graphite-diamond transition.
You will see that ELF and NCI provide complementary views of the chemical transformation. Comment.

4. (OPTIONAL) Big systems

If you are interested in big systems, you can have a look at the interactions determining the stabilization of β-sheets (sheet.xyz). Which are the main interactions? Which atoms are involved?
Now have a look at the interactions in the adenyn-thymine base pairs (AT). Remember that you may want to look only at intermolecular interactions.