Chemical bond analysis Exercises

You can download all files from
https://www.lct.jussieu.fr/pagesperso/contrera/zcam2020/zcam2020.tar.gz

Exercise 1. Identifying bonding patterns with ELF

a) Characterization of bond types. Calculate the structures (diamond, Al and NaCl) with the
following crystalline structures. Do not forget to copy the *.save repertories and calculate the ELF
cube files.

System	NaCl	Al	Diamond
SG	Fm-3m (#225)	Fm-3m (#225)	Fd-3m (#227)
Cell param (a.u.)	a=11.08	a=7.64	a=6.77
All atomic positions	Na 0.0 0.0 0.0 Na 0.0 0.5 0.5 Na 0.5 0.0 0.5 Na 0.5 0.5 0.0 Cl 0.5 0.5 0.5 Cl 0.5 0.0 0.0 Cl 0.0 0.5 0.0 Cl 0.0 0.0 0.5	Al 0.0 0.0 0.0 Al 0.0 0.5 0.5 Al 0.5 0.0 0.5 Al 0.5 0.5 0.0	C 0.125 0.125 0.125 C 0.125 0.625 0.625 C 0.625 0.125 0.625 C 0.625 0.625 0.125 C 0.875 0.875 0.875 C 0.875 0.375 0.375 C 0.375 0.875 0.375 C 0.375 0.375 0.875

- Look at Diamond isosurface ELF=0.8. Where do you obtain the basins? What is their chemical
  meaning? How many electrons do you expect in each basin?

- Look at NaCl isosurface ELF=0.7. Where do you obtain the basins? What is their chemical
  meaning? How many electrons do you expect in each basin?

- Look at Al. What does ELF=0.5 mean? Play with the ELF value around ELF=0.5 (0.5,0.55,0.6).
  Where do you obtain ELF basins? What happens at ELF=0.6? What does this mean (i.e. profile is
  steep or flat?)? How are these electrons? What model does it remind you of?

- For the three structures, justify which chemical bond is present in diamond, Al and NaCl from
  their ELF picture.

b) Analysis of a new materials. Calculate the ELF cube file for the potassium cell below. Compare
what you previously obtained with Na and Diamond. Which one does it look more alike? This is a
high-pressure structure called an electride. They are insulating metals. Try to explain this
property from the localization of electrons you have observed.

SG	Cell param	All positions
P6$_3$mmc (#194)	a=7.9608 a.u. c=10.882 a.u.	K 0.0 0.0 0.0 K 0.0 0.0 0.5 K 1/3 0.25 2/3 K 2/3 1/3 0.75

Exercise 2. Quantification

a) Atomic charges. Integrate the density basins in NaCl. What charges do you obtain? Is it what you expected? (remember you are using pseudopotentials)

b) Bond charges. Integrate the ELF basins in Diamond. Note that in this case you will need both the density and the ELF cube files! What charges do you obtain? Explain. What would you have obtained if you had integrated the density basins?

Exercise 3. Molecular crystals

a) Calculate the orthorhombic urea crystal [data are in file `urea.gen` for you to copy-paste]:

```
a= 10.516311 a.u.
c= 8.851464 a.u.
C   1.00000000   0.50000071   0.32600054
C   0.50000071   0.00000143   0.67400105
O   1.00000000   0.50000071   0.59530085
O   0.50000071   0.00000143   0.40470074
N   0.14590021   0.64590092   0.17660028
N   0.64590092   0.85410121   0.82340130
N   0.35410050   0.14590164   0.82340130
N   0.85409979   0.35410050   0.17660028
H   0.25750037   0.75750109   0.28270047
H   0.75750109   0.74250105   0.71730112
H   0.24250034   0.25750180   0.71730112
H   0.74249963   0.24250034   0.28270047
H   0.14410025   0.64410096   0.96200143
H   0.64410096   0.85590118   0.03800015
H   0.35590047   0.14410167   0.03800015
H   0.85589975   0.35590047   0.96200143
```

b) Obtain the atoms that complete the molecules in the cell (keyword MOLMOTIF) and visualize them.

c) Plot NCI (`plot_num`=19 in QE). How many hydrogen bonds do you obtain for each N? (don't forget periodicity!)