Chemical bond analysis Exercises – Only topology

https://www.lct.jussieu.fr/pagesperso/contrera/nci-exercises.html#erice2025

Exercise 1. Identifying bonding patterns with ELF

a) Download the ELF .cube files for Diamond, Al and NaCl. Visualize them with vesta or vmd.

- 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) Download the ELF cube file for the potassium. 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.

Exercise 2. Quantification

a) Atomic charges. Download the density cube file for NaCl. What charges do you obtain? Is it what you expected? (remember you are using pseudopotentials)

b) Bond charges. Download the ELF and density cube files for Diamond. 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) Download the density and rdg cube files of urea. Plot NCI. How many hydrogen bonds do you obtain for each N? (don't forget periodicity!)

b) Challenge: Download the ELF cube file for urea. Where are the lone pairs in urea and how does their position relate to the hydrogen bonds?