Chemical bond analysis Exercises

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

Exercise 1. Identifying bonding patterns with ELF

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.

Exercise 2. Identifying non-covalent interactions with NCI (NCIweb)

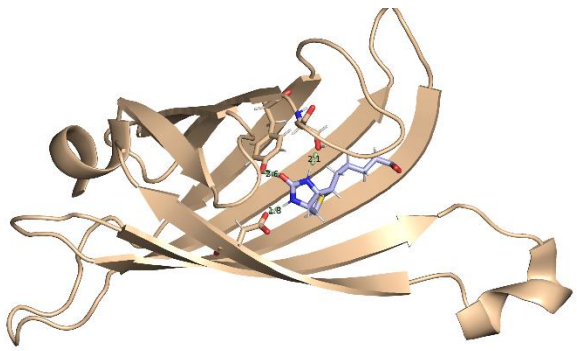
- Look at the interactions in the CB[7]-bcb supramolecular complex. What interactions are dtabilizing the ligand?

  CB[7]-bcb

- Now check the different interactions in benzene dimer and use them to understand packing in benzene crystal. Identify the localized and delocalized interactions.

  Benzene Dimer staggered
  Benzene Dimer T-shape
  Benzene crystal

- Biotin binding to streptavidin. The binding of streptavidin and biotin (vitamine H) is one of the strongest non-covalent interactions in Nature ($K=10^{13}$ M^{-1}) and a paradigm for protein-ligand interactions. Analyze pdb 1STP: Protein-Ligand 1STP



The ligand option will enable you to see the interactions leading to such high affinity. What kind of interactions are them?
How many hydrogen bonds do you find? Only some of them have been highlighted from the geometry in the picture…try to find all of them!