Visualisation d'interactions non covalentes

Visualization of non covalent interactions

Julia Contreras-García et Jean Philip Piquemal

English Abstract – This an abstract in English of the talk I will give at Visu 2013.

1 Introduction

Revealing chemical bonding (structure) and the reorganization of chemical bonds (reactivity) of any molecular system forms the undisputed foundation of chemistry. However, chemical bonds are not directly observables. Since the Hamiltonian of the system is delocalized, additional tools are necessary to: (i) describe the properties of chemically reactive systems, and (ii) extract observable information from it. Distance-dependant models have to be parameterized, which leads to many transferability problems. An adequate representation of a chemical bond as well as bond breaking/formation processes should be better provided by a physical observable defined in 3D space. The electron density meets these requirements because it is an experimental accessible scalar field, whose relationships with the system's ground-state properties can be understood from the Hohenberg-Kohn theorem. Moreover, since chemical reactions proceed by $\rho(r)$ redistributions, the methods that directly deal with $\rho(r)$ should have a particular appeal for chemists in the understanding of electronic structure and reactivity.

Moreover, molecular structure does not easily identify the intricate non-covalent interactions that govern many areas of biochemistry, including design of ligands, self-assembled materials, catalysts, drugs, and other molecular systems.

2 What is NCI ?

We have recently developed an index, named NCI, to detect non-covalent interactions in real space and they could not be easily tackled from most common topological approaches. NCI provides a rapid and rich representation of van der Waals interactions (vdW), hydrogen bonds (HB), and steric clashes as low-gradient-low-density isosurfaces.

Across numerous applications of NCI, a view of nonbonded interactions emerges as continuous surfaces rather than close contacts between atom pairs. The interactions between a deoxyadenosine-deoxythymidine pair are highlighted in Figure 1 insets (top and middle). It can be seen that NCI is able to reveal the stronger nature of N-H-O vs C-H-O interactions. Colours coding is as follows: HBs are in blue, vdW interactions in green and steric clashes in red. The large green regions are indicative of π-stacking between base-steps (Fig. 1, bottom inset).

3 NCI in big systems

Although based on the electron density and its derivatives, it only requires knowledge of the atomic coordinates, so that it is highly efficient and applicable to large systems, such as proteins or DNA. Indeed, Fig. 1 shows one such example for the different noncovalent interactions appearing in DNA.

4 Conclusion

During this contribution, we will review the basics of NCI, some of its applications from a wide range of fields, and briefly review the program, NCIPLOT, freely available for its calculation.
Special attention will be paid to the visualization challenges.

- *Julia Contreras-García : CNRS-Laboratoire de Chimie Théorique*
  E-mail : contreras@lct.jussieu.fr
- *Jean Philip Piquemal : Laboratoire de Chimie Théorique*
  E-mail : jpp@lct.jussieu.fr

Figure 1. Non covalent interactions from NCI in the B-form of double-strand of DNA. HBs between G-C and A-T and π-stacking are highlighted in the insets