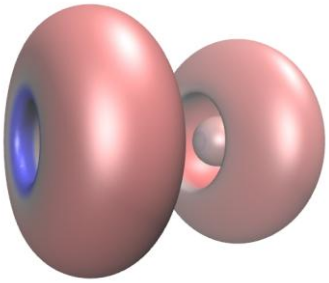
Quantum Chemical Topology for σ-hole Interactions

Julien Pilmé
Sorbonne Université, CNRS, Laboratoire de chimie théorique, Paris, France

Julien.pilme@sorbonne-universite.fr

In the first part of this talk, I will present an overview of quantum chemical topology (QCT) descriptors used to rationalize the *σ*-hole bonding schemes, with a focus on Bader's QTAIM and ELF approaches and the Interacting Quantum Atoms (IQA) methodology[1], as well as analyses based on the conceptual DFT.[2] I will notably show how the effects of both primary and secondary interactions can be related to the stability of some complexes, with particular focus on the coulomb and exchange contributions.

In the second part of the talk, our strategy to evaluate spin-orbit coupling (SOC) effects on halogen-bond interactions within quasirelativistic wavefunctions will be discussed. I will show how the QCT approach can provide a straightforward way to highlight SOC effects on classical paradigms. [3, 4, 5]



Dual Descriptor(DD) of the conceptual DFT mapped onto an ELF isosurface (ELF = 0.65) for I_2 molecule.
Color code: blue DD>0 and red DD<0

References :
[1] Syzgantseva, O.A.; Tognetti, V.; Joubert, L. *J. Phys. Chem A* **2013**, *117*, 8969-8980
[2] Morell, C.; Grand, A.; Toro-Labbé, A. *J. Phys. Chem.* **2005**, 109, 205-212
[3] Pilmé, J.; Renault, E.; Ayed, T.; Montavon, G.; Galland, N. *J. Chem. Theory Comput. Letter* **2012**, 8, 2985–2990
[4] Sarrr, S.; Graton, J.; Montavon, G.; Pilmé, J.; Galland, N. *Chem. Phys. Chem.* **2020**, *21*, 240-250
[5] Graton, J.; Rahali, S.; Le Questel, J-Y.; Montavon, G.; Pilmé, J.; Galland, N. *Phys. Chem. Chem. Phys.* **2018,** *20*, 29616-29624