Does the Intra-atomic Deformation Energy of Interacting Quantum Atoms Represent Steric Energy?

Invited for this month’s cover picture is the group of Paul L. A. Popelier from Manchester Institute of Biotechnology (UK). The cover picture shows the quantum topological atoms in a configuration of the complex HF···OH$_2$, where F is green and O is red. Read the full text of their Full Paper at 10.1002/open.201800275.

Who designed the cover?
Popelier and Symons.

Does the research open other avenues that you would like to investigate?
Yes; the impact of interacting quantum atom (IQA) energies on drug design. In particular, topological atoms are space-filling, thus there are no empty regions of space. This fact could change the standard view on how a drug (ligand) interacts with an enzymatic pocket.

What aspects of this project do you find most exciting?
That all the parts of IQA now fall into place. The wider context of this work is that all chemical phenomena follow from an interplay of four primary energy quantities: steric, electrostatics, exchange interaction and dynamical correlation. Other work has shown how these quantities make contact with classical potentials, but the current work and sister paper$^{[1]}$ establish the intra-atomic energy (and particularly the kinetic energy contribution) as a measure of steric repulsion. Secondly, it was exciting to finally find a rigorous explanation as to why hydrogen is often represented as not producing steric hindrance.

Is your current research mainly curiosity driven (fundamental) or rather applied?
Definitely curiosity driven. The work of an older sister paper$^{[1]}$ was extended, out of curiosity, to more general molecular orientations, beyond the molecules approaching each other always along the line, linking the two non-hydrogen atoms. The driving question was: is the mapping of sterics and short-range interatomic repulsion to topological deformation energy still valid for less artificial approaches? The answer is “yes”, and the steric nature of hydrogen was thereby properly explained.

[1] A. L. Wilson, P. L. A. Popelier, J. Phys. Chem. A 2016, 120, 9647.