Research interests

Magnetically induced current density. When a molecule is exposed to an external magnetic field its electrons are forced to move around parts or around the entire molecule, giving rise to a magnetically induced current density. In cooperation with researchers from the Gent Quantum Chemistry group, we developed an in-house FORTRAN code for calculation of the induced current density using modern ipsocentric methods. In a recent development, we use the Paraview program to visualize the calculated current densities. Our code provides several possibilities to calculate, visualize and integrate the current densities. The magnetically induced current densities provide the information on how electron charges move in molecular systems placed in magnetic fields. In an implicit form, the current density gives a measure of the extent of electron delocalization. Therefore, the current density is widely used to study chemical phenomena based on electron delocalization. We use the current densities mainly to study the aromatic behavior of molecules. In such studies we also employ different aromaticity indices, calculated using several independent theoretical methods (DFT, graph theory,…). We have strong collaborations in this area with theoretical chemistry groups in Gent, Vigo, Groningen and Kharagpur.

New bonding concepts. We analyze new bonding mechanisms, such as "charge-shift bonding". Our main tool in these studies are modern Valence Bond (VB) theory methods implemented in the XMVB program. We also employ recently developed approach combining Quantum Monte Carlo (QMC) methods, which are known to be very accurate, with VB methods which have significant interpretative capabilities. In this filed we have collaborations with theoretical chemistry groups in Paris and Jerusalem.

Theoretical and computational investigation of electronic properties and reactivity. Widespread quantum chemistry computational methods are employed for the analysis of intramolecular bonding, intermolecular interactions and reactivity. Of particular interest is the study of electronic properties of polycyclic aromatic systems which in their ground electronic state have two π-electrons unpaired and prefer to exist in a paramagnetic form. Reactions in organic, inorganic chemistry and biochemistry are studied, from both kinetic and thermodynamic aspects.

Chemical graph theory. Electronic properties, aromaticity and reactivity of polycyclic aromatic molecules are studied by means of graph theory indices. In our previous studies, we investigated the graph-spectrum-based invariants (e.g. Laplacian energy, Estrada index,…). Understanding of the dependence of these molecular descriptors on main structural features of molecular systems is of crucial importance in their applications in quantitative structure-activity and structure-property relationship (QSAR and QSPR) methods. Our faculty has world-renowned scientists in this field.