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The dual descriptor and its possible use for a rational design of novel molecules with importance in nanoscience and nanotechnology

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Abstract

The growing importance of nanoscience and nanotechnology implies not only the development of new experimental techniques for characterization of nano-structures, but also the development of new processes of synthesis in order to make easier the production of novel compounds that are expected to be generated at industrial scales. However, getting a more rational insight about reaction mechanisms that permit the synthesis of these final products is still an issue of interest in basic science and hence new theoretical and experimental procedures are needed to provide this type of information. Quantum chemistry is not an exception because it has demonstrated to be very useful to shed lights about the description of several types of molecular structures. In particular, a key aspect is the reactivity because it allows identify those sites on a molecule that present a major trend to form or destroy a chemical bond, thus turning the original molecule into another one with expected or unexpected properties and applications. Different theories based on Quantum Chemistry are able to provide conceptual tools to understand chemical transformations. One of these theories is called Conceptual Density Functional Theory [1] which provides global, local and non-local reactivity descriptors. In particular, the Conceptual DFT has given rise to the so called dual descriptor which is able to reveal sites susceptible to receive nucleophilic and electrophilic attacks, and although this descriptor is still under improvement [2] this descriptor has demonstrated to be a robust tool to understand reaction mechanisms [3]; it is expected that the Conceptual DFT can be used in assisting synthesis of novel compounds and for understanding reactivity of different structures like fullerenes [4]. This talk will be focused on this local reactivity descriptor and its possibilities to be used as a guide for synthesis of new compounds within the field of nanoscience.

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[4] J.I. Martínez, J.L. Moncada, J.M. Larenas, "The dual descriptor to measure local reactivity on Buckminster fullerenes: an analysis within the framework of conceptual DFT", *J. Mol. Model.*, **2010**, *16*, 1825.