Corentin Boilleau et al., J Phys Chem Biophys 2017, 7:4(Suppl)
DOI: 10.4172/2161-0398-C1-025

Theoretical study of magnetic properties in redox-active ruthenium complexes

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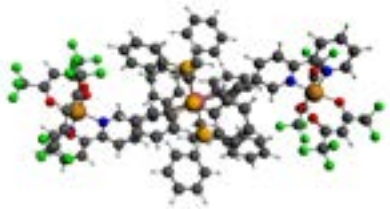
Due to the slowdown of the information technology development, a great challenge of present-day applied science is to develop new electronic devices at the molecular scale. Indeed, molecular spintronic offers great potential multifunctional molecules performing new properties or operations unreachable by conventional semi-conductor technology. This project takes place in this quest of tomorrow's technologies conquest in the new field of molecular spintronic. The goal is to provide multifunctional compounds made from bricks with remarkable properties for storage or manipulation of information across a single molecule. This work use an uncommon strategy based on redox properties of ruthenium compounds associated with magnetic centers in order to obtain a device allowing a modulation of the magnetic properties. The aim is to study the inter-molecular interactions, to understand the interplay of the components in view of obtaining their synergistic working mode. Considering the crucial role of the electronic correlation in magnetic systems and the strong geometrical and electronic coupling existing between the different functional elements, modeling of such systems is a tough task. A correct description of these systems requires taking into account the couplings between the subunits. The nature of the interactions studied the presence of transition metals and the need for investigation of both ground and excited states suggested the use of post Hartree Fock methods. But, considering their computational cost and the size of our systems, they are here prohibited. Therefore, the use of DFT with hybrid functional is suitable. Standard and broken symmetry calculations have been performed to determine the magnetic coupling. The supramolecular assembly proposed present efficient switching properties allowing the realization of logical functions. Depending on their composition, shape, physical and chemical properties, they can be used as data processing devices (molecular wires, transistors, circuits) as information storage devices (molecular switchers) or as molecular machines.



Biography

Corentin Boilleau has his expertise in electronic structures and magnetic properties. He completed his PhD and then joined Vincenzo Barone's laboratory in Pisa for two years. He also joined Karine Costuas in Rennes for one year in order to study ruthenium based compounds using DFT methods and model Hamiltonians. Currently, he works at Institute of Physics in Warsaw where he obtained a grant for three years to carry out a study on multifunctional compounds allowing a modulation of their magnetic properties.

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