The slowdown of the information technology development spawned the need to look for an alternative ways of data storing and treating. Nowadays a great challenge for the applied science appeared: is to develop new electronic devices at the molecular scale which may be an alternative to semi-conductor technology. The present work addresses this challenge offering molecules of great potential in order to reduce the size of devices to the nanoscale. Above project is part of trends in designing of tomorrow's technologies in the new field of Molecular Spintronics.

Spintronics is a technology taking advantage of a quantum property of electrons called spin. Electron spin can be compared to the rotation of a planet or a spinning top around its axis. An electron can rotate in the clockwise or counter-clockwise direction which can be illustrated as a direction given to the spin, respectively "up" or "down". Spin gives electrons their magnetic properties, influencing their behavior under the action of magnetic field. Different directions of electron spin can be used to encode information as the binary code used in digital communication, "down" mimicking the "0" and "up" the "1". Spintronics can therefore open up a new generation of devices that combine conventional microelectronics with spin-dependent effects, overcoming the limitations of today's electronics such as speed limitation and energy consumption. The main challenge is to be able to efficiently control electron spin, turning "up" or "down" when needed, and to keep electron spin in the desired direction.

The strength of Multifunctional Molecular Devices is the diversity of their industrial applications. The development of high performance magnetic materials improves efficiency of electric vehicles, industrial motors and wind generators, contributing in energy saving. Furthermore, the advanced magnetic recording media and magnetic sensors leads to substantial electric power saving in data storage for cloud computing. Moreover, miniaturization to the nanometric scale to have a positive ecological impact, decreasing the waste production and Greenhouse gas emissions.

The goal of the present project is to propose, through the theoretical prediction, new Multifunctional Molecular Devices (MMDs) offering a reversible switching (from "0" to "1" and from "1" to "0") under the action of light or an electric potential. These MMDs are constructed using single molecules as elementary bricks. The resulting assembly accumulates the properties of each elementary unit providing the desired function. The developed compounds concern data processing devices (e.g. molecular wires, transistors, circuits) and information storage devices (molecular switchers) in quantum computers. In addition to the applications dedicated to molecular spintronics devices target systems can potentially be used in detection or biotechnology (e.g. high resolution imaging). Moreover, the understanding of the working mode of Multifunctional Molecular Devices and identifying promising candidates will allow us to lead experimentalists in their synthesis to reach mass-production.