Popular science description

The long term objective of the proposal is exploration and development of the future perspectives towards data processing (recording, storage and read-out) and quantum computing. As the amount of potential data to be processed is still increasing, the optimum approach towards the above goals may rely on miniaturization of the mediating tools. Thus, the targets should be located among such small objects as molecules or even single atoms. Nowadays, considering the magnetic or optical data processing, the pioneering works are performed along two channels: (*i*) exploitation of several known pre-selected mediating molecules integrated with suitable surfaces, fulfilling very strict conditions or (*ii*) studies on the embedding of molecules or molecular aggregates embedded in the crystal matrix in very specific unique conditions. Although the results are promising, plenty of obstacles still remains to overcome. This creates a strong continuous need of elaboration of new synthetic strategies towards underlying materials. One of the main problems is a small degree predictability of local molecule-surface or molecule-molecule interactions. This is an individual problem, to be separately recognized for each examined system.

Along the above line, this proposal is focused on the searching for the new multicomponent molecular systems that could be, in the future, suitable links towards implementation of the functionality based on switchable properties involving charge transfer (CT) and electron transfer (ET), structural non-rigidity and spin non-rigidity, magnetic properties, and optical properties. The concepts for multicomponent molecular systems has emerged during the recent decade, along the use of the *building blocks approach* and *molecular tectoniques* for the construction of *multifunctional molecular magnets*, *luminescent molecular materials*, or *molecular co-crystals* and others. Going to details, this proposal aims to approach towards recognition and exploitation of the predictable block molecular arrangements, exploiting (*i*) the coordination and/or supramolecular architectures offering the areas pre-programmed for exchangeable hosting of various chemical moieties and (*ii*) chemical species with specific distribution of electronic density, for shaping the required structure and properties. It will deal with (*i*) organic-inorganic hybrid co-crystals, (*ii*) molecular core-shell crystalline composites, and (*iii*) polynuclear multimetallic coordination architectures, all based on specially selected molecular components. Starting from the typically observed magnetic and optical properties, it is intended to develop the combined interplaying schemes for-more-than-one-channel manipulation, which should increase the operational space for the data processing.