

Description for the general public

Nowadays, there is considerable attention paid to the search for new functional materials that would enable the construction of **modern memory disks with high data density**, components of **quantum computer architectures**, or materials applicable in the generally understood **spintronics**, i.e. the section of electronics based on the use of spin instead of the traditional electron charge. Promising candidates that can offer the desired physical properties for these purposes are so-called **Single-Molecule Magnets (SMMs)**, the first representatives of which were discovered around 25 years ago. SMMs consist of paramagnetic complexes of transition metal and rare earth (lanthanide) ions, isolated in the supramolecular framework or embedded in the coordination networks of various dimensionalities, that reveal a magnetic hysteresis loop below the so-called blocking temperature (T_B). Surprisingly, this hysteresis is not the result of magnetic interactions leading to the spin ordering and formation of domains, as is the case of classical magnets known from everyday life. This magnetic hysteresis has a purely molecular basis, originating from the specific electronic structure of metal ions placed in the crystal field of ligands. Therefore, we can treat such isolated molecules or ions as real miniature magnets. Their potential applications are limited by time (the so-called magnetic relaxation time, abbreviated as τ) during which a given molecule is able to maintain its magnetization after removing the previously applied magnetic field, and by extremely low temperatures below which the described magnetization blocking phenomenon can be effectively observed. If we could develop new families of SMM molecular systems with extended τ times leading to the magnetic hysteresis observable at room temperature, miniaturization of devices and electronic memory at the level of isolated chemical molecules could be achieved!

After many years of intensive experimental and theoretical research, we have extensive knowledge on the so-called static properties of the electronic structure that are mandatory to observe the blocking of magnetization and the construction of SMM-type materials with potentially huge spin reorientation barriers and the resulting very long magnetic relaxation times. However, relatively little is known about the exact course of **magnetic relaxation processes caused by lattice vibrations**, i.e. spin-phonon interactions in real molecular nanomagnets which are always arranged in the specific crystal lattice. With the above in mind, the main goal of the project is to comprehensively simulate the time and paths of magnetization relaxation induced by vibrational couplings within the crystal lattices of the selected molecular nanomagnets. As the SMM objects for all our considerations, we will select candidates from the unique family of **lanthanide-based single-molecule magnets formed in coordination frameworks** built of magnetically anisotropic lanthanide ions and diamagnetic transition metal complexes. Focusing on this type of SMMs, we will address the non-trivial, yet completely unexplored, the question of how the coordination-network-type crystal lattice affects the slow magnetic relaxation phenomena of incorporated lanthanide SMMs. For achieving this goal, we plan to use a number of **relativistic 'ab initio' methods based on multi-configurational quantum-chemical calculations (e.g. CASSCF) as well as those using the theory of density functionals (DFT)** to obtain effective parameters of the Hamiltonian responsible for the **spin-phonon coupling**. Then, by solving the quantum master equations for the reduced density matrices of the studied systems, we will obtain information about the time evolution of magnetization which will be confronted with the performed experimental characterization used as the verification tool. Thanks to the theoretical calculations carried out, we plan to indicate the most effective paths leading to the loss of magnetization and eliminate them by proposing potential modifications for the tested systems. We are convinced that this type of research can contribute a lot to understanding the exact mechanisms governing the spin dynamics of SMM systems and lead to the future development of compounds with significantly improved magnetic characteristics that can be successfully used in the construction of the future extremely high-density memories and high-performance spintronic devices.