**DESCRIPTION FOR GENERAL PUBLIC**

The exponentially growing amount of computer produced data causes the growing demand on capacity of computer hard drives. It is obvious that for new generation of disk drives not only optimized materials are needed but also new concepts for data storage. At present the magnetic hard disks need few hundred grains of typical 10 nanometers in size to store one bit. The further decrease of number of grains or diminishing their diameter to store one bit can affect the signal/noise ratio and in result lead to loss of information. Therefore, scientists are looking for new ideas for magnetic storage media. One of the ideas it is to graft molecules with internal magnetic moments (single molecule magnets – SMM) on a surface. The array of grafted molecules constituting a regular lattice could be prototype of the magnetic storage device. In this context the novel hybrid structures involving two-dimensional nano-materials (2D-NM) and single molecule magnets (SMMs) are considered to be promising candidates for novel generation of devices. Two-dimensional systems, such as graphene, hexagonal boron nitride, planar dichalcogenides (e.g., MoS2), exhibit intriguing properties, and at present they are considered worldwide as the most promising candidates for future applications in the whole plethora of fields including nano-electronics, optoelectronics, spintronics, and novel smart materials. The functionalization of these layered systems with SMMs can lead to required functionalities exhibiting by the hybrid 2D-NM/SMM structures and lead to tunable array of magnetic nano-objects on a surface of a system, and then to the novel spin-based technologies. Inspired by the intriguing results of the first studies, the experimental research in this field is blooming and presently three European Research Council projects *(GraM3*, *MAGMETALS*, and *MOLNANOMAS*) are digging for novel spintronic functionalities in these hybrid systems. However, in spite of huge experimental effort the observed phenomena are not completely understood.

In the present proposal, we indent to perform extensive theoretical studies of: (i) the stability of such structures, (ii) the nature of interactions between the localized spin in SMM and 2D-NM to which the molecule is grafted, and (iii) mutual interactions between SMMs' magnetic moments. Further, we would like to find out how the magnetization of SMMs can be modified through external factors such as electric field, static magnetic field, electromagnetic radiation (light), charge and spin current flowing through the adsorbent to which SMMs are grafted. These studies should shed light on the physical mechanisms governing the magnitude and anisotropy of magnetization in SMMs and pave the way for chemical engineering of such hybrid structures. We hypothesize that the multi-scale theoretical tools developed in this project provide: (i) necessary understanding of the physical mechanisms that determine the properties of the 2D-NM/SMM hybrids, and (ii) reliable accurate quantitative predictions for experimentally investigated structures, which both allow us to select the most suitable hybrid structures for future spin-based technologies.

This proposal describes novel and ambitious scientific research that goes beyond the standard calculations of material properties and will enrich the theoretical condensed matter physics, quantum chemistry, and materials science. We will develop the computational scheme that allows for realistic modeling of the 2D-NM/SMM hybrids in geometry close to the experimentally investigated structures. The studies to be performed in the planned project are, therefore, important not only for the basic physics, chemistry, and materials science, but have meaning for future nano-electronics and nano-spintronics that will determine the further development of the 'information age' of our civilization.