The main goal of the proposal is to work out the synthesis procedure of hybrid thin silica films activated by metal ions and magnetic molecules. Then their synthesis and thorough investigation of physical properties.

The completely pioneering materials proposed here have great application potential. According to my best knowledge such materials have not been investigated or prepared before.

The materials that are considered here have double layer structure. It consist of base silica layer with bounded active molecules and mesoporous layer with hexagonally arranged channels, oriented perpendicularly to the substrate. Each channel contains single magnetic molecule or metallic ion on the bottom. For such a structure active groups do not interact with each other - they are separated by silica walls. Therefore it is possible to obtain separate bistable magnetic units (in the case of films activated by molecular magnets) with diameter up to 8 nm. Moreover, magnetic units are distributed regularly in the layer.

The first layer of materials proposed here is silica containing anchoring groups, appropriate for ions or molecules. The layer is deposed directly on the substrate. The role of anchoring groups is to bound molecules or ions during activation process. On this layer next mesoporous silica layer is deposed. This second layer contains hexagonally arranged pores with amorphous walls, oriented perpendicularly to substrate, with diameter up to 5 nm (depending on surfactant and synthesis conditions). After deposition onto first bounding layer, the second layer will create honneycomb-like structure. Due to low diameter of silica channels, it is possible to obtain single anchoring group in the channel. Of course such a synthesis is a statistic process, so there is a possibility of finding more than one anchoring group inside a channel, but low pore diameter can assure activation of channels by single magnetic molecule (Mn_{12} molecule has lower diameter, but comparable to pore diameter).

It is planned activation of obtained layers by metal ions: silver and copper and by single-molecule magnets - Mn_{12}. It is worth noting that the material activated by molecular magnets has the highest applicational capability. Films activated by metallic ions can be obtained in much easier way and their investigations are easier to interpretation. The synthesis of metal containing samples has purely basic character. The results obtained in the previous stage (distribution of anchoring groups and their activity) can be treated as a starting point to preparation of molecular magnets containing films.

It is unquestioned advantage that applicant has a great experience in deposition of thin silica layers. She was a main contractor in a grant concerning SBA-15 silica materials. Metal containing SBA-15 silica is also a subject of her Ph.D. thesis. The procedure will be worked out on the base of earlier experiences and preliminary research and on the base of literature data.

The research proposed here will be divided into two stages: optimisation of synthesis route and characterisation of obtained (and verified) materials.

At first stage the synthesis procedures of thin films with assumed structure will be worked out. It is planned to use a several substrates (silicon wafers, glass, mica, etc.), what can facilitate the structure's optimisation. At least two surfactants will be used to obtain different pores diameters: 2.5 nm (CTAB) and 4.5 nm (P123). The possibility of pores diameter tuning allows for obtaining key feature of proposed material: each pore is activated by distinguished molecule. Next, the samples will be prepared according to worked out procedures. The hybrid thin films obtained in a previous stage will be examined in terms of microscopic and molecular structure. This will be done by a series of basic research. On the base of the results previously obtained, the synthesis routes will be optimised to obtain the layers with exactly assumed properties. This procedure will be repeated iteratively as long as the assumed results are obtained.

The atomic force microscopy (AFM) allows for estimation of surface quality and roughness of obtained layers.

Transmission electron microscopy (TEM) allows for direct observation of the structure. The research can examine structure of pores and their arrangement (are they arranged hexagonally and perpendicularly to substrate?). It should be noted that TEM investigation will be possible thanks to innovative method of free-standing thin films obtained, which was worked out by the nanotechnology group with applicant participation.

Small angle X-Ray reflectivity research, aside from basic structural data (obtained also in TEM observation) allows for calculation of porosity (characteristic for porous materials plateau of total external reflection with strong dip at critical wave vector) and thickness of layers (calculated from distance between Kiessig fringes).

Wide angle X-Ray reflectivity can give information about eventual excess of doping agent.

Verification of the molecular structure is possible by use of Raman spectroscopy supported by DFT simulations. The testing procedure proposed here has been tested with good results on SBA-15 silica powders containing metal ions. On the base of numerical simulations it is possible to find characteristic Raman peeks, occurring only for certain bounds. Obtained experimentally Raman spectra are compared to the theoretical spectra for considered and reference samples. By this juxtaposition it is possible to determine the molecular structure of molecular groups occurring in the samples. It should be noted that applicant posses a numerical models for a part of proposed materials.

As a result of first stage of research we assume to get at least three types of hybrid thin silica films (containing silver, copper and Mn_{12}).

In the second stage obtained materials will be investigated in order to determine their physical properties by a series of basic research.

Electrical properties will be examined with the help of AFM microscopy (conductivity in direction perpendicular and rectilinear to substrate) and broadband dielectric spectroscopy (dielectric properties).

Magnetic properties will be measured by SQUID magnetometry (thanks to the technology of free-standing thin films).

Deliverable of the project will be novel materials with complete characteristics, obtained thanks to interpretation of basic research results. It is also expected to publish at least two articles in journals with high impact factor.

The main reason of choosing this subject was great application capability of proposed materials. Utilitarian approach to projects implementation allows for logical and coherent planning of methodology, in spite of fully basic character of the project.

Proposed approach to thin films synthesis follows Eric Drexler postulate: synthesis of nanomaterials should be planned in such a way, that molecules assembles by itself, creating nano tool or material with desired properties. In this case the hybrid thin films properties can be used mainly in microelectronics and molecular electronics.

Obvious domain for application can be computer memories. The material can be used as a memory cell with enormous density (capacity). Each silica channel, arranger regularly in the form of thin film, can be treated as a separate bistable magnetic unit (molecular magnet in each pore). The polarisation of such a unit can be read and write with the help of magnetic field (e.g.

scanning tip). Taking under consideration the films structure it is possible to obtain memory cell with diameter from 5 to 8 nm. It gives up to $4 \cdot 10^{10}$ bits in 1 mm^2 of the film, what is really unusual value.

The thin films proposed here can be used also as a converting units in molecular Hopfield-type neurons. The research group, the applicant is engaged in, is working on this concept currently. This new technology development leads to hardware implementation of artificial neurons based on molecular techniques. Proposed solution is an enlarged model of the Ising model. Considered technology can significantly influence research and application areas in a long-term perspective. For instance a straightforward application seems to be a content addressable associative memory (CAAM). This kind of memory, implemented on the molecular scale, offers both high capacity and instant access, which in turn opens up new and unprecedented possibilities for artificial intelligence. It is easy to realise that molecular CAAM, with all kind of patterns and ease to learn new ones, can move forward the artificial intelligence research.

The technology, being a subject of the proposal, will also offer new opportunities for solving multi-criterion optimisation problems. Such problems, involving more than one objective function to be optimised simultaneously, what can be extremely difficult to solve. Problems of this type can be found in mathematics, engineering or economics. Vector optimisation problems arise, for example, in decision making, statistics, functional analysis, approximation theory, multi-object programming or cooperative game theory. As it was proved, the Hopfield networks are very efficient in solving such problems, but also disappointingly slow. As a result, solutions can be found at the expense of computational time. When using a real parallel system, like the one described in the proposal, a solution can be found instantly.

Apart from applicational potential, proposed materials are very interesting from the scientific point of view. None of similar solution has ever been proposed in literature. Thanks to use of silica matrix with proposed structure, it is possible to investigate properties of single molecular magnets and single molecules (it is possible to obtain ions or molecules groups, depending on concentration of anchoring groups). It is commonly known non-stability of Mn_{12} molecules with the contact with different substrate. But as we have observed, the properties of isolated Mn_{12} bounded to silica matrix do not change. In the present project it is possible to examine the limiting situation: single pore contains isolated molecule. In the case of finding stable material, the species can surely find commercial application, but also it is possible to continue investigation within a framework R+D project.