The main aims of the project are synthesis, characterization, theoretical description, and computational modeling of properties of compounds based on transition ions (3d/4f) exhibiting properties of molecular nanomagnets (MNM) optimized for applications in quantum computers of the future. Experimental work will by supported by computational modeling allowing to predict the desired properties using semiempirical as well as quan-tum chemistry methods (*density functional theory* (DFT) and *ab initio*). This will enable rational design at the molecular level of novel MNM with predetermined properties taking into account the sources of magne-tic anisotropy and factors controlling the height of the energy barrier for magnetization reversal. An aim of theoretical work is also explanation of unsolved or controversial aspects, among others: forms of generalized spin Hamiltonians for single 3d/4f metal ions and exchange coupled clusters, role of higher-order terms in generalized spin Hamiltonians for MNM, symmetry of *multispin* and *giant-spin* Hamiltonians, role of spin-orbit coupling in description of MNM. The **research hypothesis** assumes that explanation of these aspects and apt choice for synthesis of 3d/4f ions and ligands aided by computational modeling allow obtaining MNM with supramolecular architectures exhibiting ligands' coordination that stabilizes the ground state being maximally favorable for optimization of properties for practical applications in quantum computers of the future.

Research will be carried out by international and interdisciplinary group of chemists and physicists and in close collaboration between experimentalists and theorists. International experimental (Japan) and theoretical (Turkey) studies will be possible due to an agreement with our colleagues on unpaid collaboration leading to joint publications. **Experimental part** includes synthesis and characterization of new compounds. Based on initial choice of quinoline unit as the basic building block for condensation with suitable aldehydes /ketones, we plan synthesis of several Schiff base ligands as precursors of new metallosupramolecular architectures with potential properties of MNM. X-ray diffraction techniques will serve for determination of coordination of metallic centers, ligands' conformation and ways of formation of three-dimensional supramolecular lattices in coordination compounds. Characterization of synthesized compounds will be carried out using various complementary techniques: optical spectroscopy - measurements of emission and absorption, electron magnetic resonance (EMR) - measurements in X and Q bands at various temperatures, and variable temperature measurements of magnetization and magnetic susceptibility in *dc* and *ac* magnetic field and at various field frequency using SQUID magnetometer. EMR studies at high magnetic fields and frequencies (HMF-EMR) and in wide range of temperature and pressure have innovatory character and go beyond the existing knowledge. The HMF-EMR measurements will be carried out by Japanese researchers using unique equipment, which is not available in Poland. **Theoretical part** includes computational modeling geared towards the aims specified above. For description of the properties of the constituent 3d/4f ions forming MNM molecules, we will utilize the crystal field (CF) theory and the spin Hamiltonian (SH) theory, and for the exchange coupled clusters - the *giant* and *multispin* Hamiltonian approaches. For computational modeling of the spectroscopic and magnetic properties we will utilize semiempirical methods and quantum chemistry methods [DFT/*ab initio*].

Comprehensive study of spectroscopic and magnetic properties, combined with theoretical analysis of results, is an innovative approach, since hitherto studies have been conducted separately, whereas comparison of data provided by both complementary methods was severely hampered because of usage of disparate theoretical as well as experimental parameters. Quest for novel MNM is innovatory and goes beyond the existing knowledge. The project has great potential importance also because (a) in viewthe phenomena observed in the very high magnetic fields used in HMF-EMR have not yet been fully explored, (b) the aspects mentioned above are not solved or controversial. The subject is a leading one worldwide due to the phenomenon of the macroscopic quantum tunneling of magnetization (QTM) and important potential applications, e.g. in quantum computers of the future, nanotechnologies and spintronics. The project is of cognitive nature and serves advancement of fundamental knowledge about MNM and development of alternative methods of MNM synthesis. Characterization of spectroscopic and magnetic properties of synthesized MNM compounds, in correlation with crystal structure, as well as computational modeling and prediction of these properties will enable rational design of novel MNM. Modeling of the properties of MNM systems, depending on the external factors will allow deepening fundamental knowledge concerning the relationships between crystallographic structure and experimental parameters. Synthesis and characterization: structural, spectroscopic, and magnetic of the potential MNM, using the number of complementary measurement techniques, including the modern HMF-EMR techniques, will provide data for computational modeling and prediction of properties of selected MNM complexes, have innovatory character, not only due to novel compounds being synthesized, but moreover due to comprehensive linking of theoretical, experimental, and computational studies. Cooperation of experimentalists and theorists enables synergy, which may lead to new significant discoveries essential for the progress of science and practical applications of MNN.