New Materials with Electronic and Magnetic Correlations

Materials, in which the extraordinary effects of quantum mechanics can induce unique and unexpected behaviors, are the key to revolutionizing the future energy and information technologies. This proposal aims to establish a strong research program at Gdansk University of Technology (Poland) by collaborating with Princeton University (USA), Louisiana State University (USA) and Tokyo University (Japan), with the goal of addressing challenging issues to discover new strongly correlated materials with exotic physical properties. By applying our fundamental understanding of the correlations among crystal structures, physical properties, and chemical bonding, we will synthesize and characterize the novel materials with the aim to understand how magnetic and superconducting properties are related to their chemical composition and atomic structure in a quantitative approach and facilitate the technological applications in a long term. In particular we will focus on new materials, both oxides and intermetallics, which exhibit interesting properties such magnetic ordering or superconductivity.

One of the aims of this project is to target “molecular” trimer systems in oxide materials. The importance of spin-orbit coupling (SOC) to generate the electronic ground state in 4*d*/5*d*-based compounds has emerged and many new novel routes to a host of unconventional physical states have been revealed, for example, quantum spin liquids, Weyl semimetals, and axion insulators. This project aims to design, synthesize, and characterize the molecule-based inorganic 4*d*/5*d* transition metals oxides, with the goal to understand how magnetic properties are related to their chemical composition and atomic structure. Currently, major experimental and theoretical efforts have been solely undertaken to search for novel spin-orbit coupling systems in the various d^5 system with $S = 1/2$. We will investigate the structure-magnetism interactions in new $Ba_4MIr_3O_{12}$ oxide compounds by combining experimental results and chemical bonding & molecular orbit diagrams.

A parallel objective of the project is to continue our previous, successful HARMONIA project. However, we will broaden our search for the superconductivity in new endohedral M cluster (M = Al, Ga, In). One of the chemical views to increase the occurrence of new superconducting materials is to posit that it carries out in structural families. Thus, another primary goal of this proposed research is to apply the structural connection for the interpretation and prediction of other possible new superconductors adopting to the similar framework. We will also continue our effort in searching antiperovskite compounds focusing on Ru, Os and Ir based materials.