Project title: Future permanent magnets from design

Project author: Mirosław Werwiński

The aim of the project is to develop a new generation of magnetic alloys for application as permanent magnets and study of influence of chemical composition on their magnetic and electronic properties.

The motivation to undertake the above research is the search for new hard magnetic materials containing no rare-earth metals as the replacements for commonly used neodymium magnets. These searches are motivated by the volatile prices of rare earth metals and the risk of their resources being exhausted in the long run. The first-principles calculation results obtained in the project will become a signpost in the development of a new generation of permanent magnets.

The project focus on iron-, cobalt-, manganese- and cerium-based materials and their alloys with 5d-elements. In the project, the selected materials are computer-modelled in an atomic scale using the quantum-mechanical computation methods, called the first-principles calculations. In the project we calculate the intrinsic properties of the bulk materials critical for permanent magnets applications, which are the saturation magnetization, magnetocrysalline anisotropy energy (intrinsic anisotropy) and Curie temperature. The project members closely collaborate with partners from the Department of Physics and Astronomy of Uppsala University in Sweden. The computational grant at Poznań Supercomputing and Networking Center (PSNC) ensures an effective implementation of the computational tasks.

The final effect of this project will be the result of broad computational studies which will identify the most promising candidates for the rare-earth free permanent magnets applications from the group of the considered alloys. We expect that the most promising candidates predicted from *first principles* can be synthesized and exhibit advantages over the existed rare-earth free materials. Furthermore, the improvement in general understanding of the problem will allow for develop of the new strategies for discovering the new permanent magnets.