

Nanostructures containing transition metals have very interesting properties from the point of view of basic research, as well as have a large potential of applications in nanotechnology. The iron-silicon compounds discussed in presented project are very good examples of such materials. These systems located at a suitable surface can self-assemble to form ordered nanoclusters and nanowires. Due to the high electrical conductivity and high chemical stability, these materials may be used to create electrical connections in new electronic devices and due to their magnetic properties they are considered as very promising candidates for applications in magnetic, spintronic and logic devices. Low dimensionality of these systems can also influence the superconducting properties as it is observed in FeSe monolayer placed on SrTiO₃ substrate. Significant enhancement of the critical temperature makes the technological exploitation of similar systems possible in the future. The development of theoretical method and description of the properties of proposed structures seems to be of essential importance. Having theoretical models allow us to study new phenomena such as the unconventional superconductivity in the iron-based superconductors.

However, with such a large miniaturization not fully understood size effects start to play an important role. The main problems we face are the temperature induced destabilisation of systems structure, effective dissipation/drain of heat and strong modification of the elastic properties that determine the strength of the material. All these properties are directly related to the way in which the individual atoms move in the crystal, and the energies of such movements.

The aim of this project is to conduct a comprehensive research of structural and dynamic properties of a selected group of nanomaterials using both theoretical and experimental methods. Our research group from the Institute of Nuclear Physics, Polish Academy of Sciences specializes in the calculations of material properties using a so-called first principles methods, based on the basic laws of quantum mechanics and statistical physics. We have the skills and computer software that allows us to determine the basic characteristics such as crystal lattice parameters, electronic structure, magnetic moments, elastic and dynamic properties of the tested materials. Even the most advanced computational methods need to be verified by appropriate experiments, which in turn require theoretical description of the correct interpretation of measurement results. In the project we will make use of the data measured at the European Synchrotron (ESRF) in Grenoble, at the German Electron Synchrotron (DESY) in Hamburg, and at the Swiss Federal Institute of Technology in Lausanne (EPFL). Samples for measurement will be created *in situ* (inside the measuring apparatus) during the experiment by a group from the Karlsruhe Institute of Technology. Such close cooperation between our groups is a prerequisite for a fruitful research on complex nanostructures and guarantees achievement of research goals. All these systems are characterized by complex couplings between their crystal structure and electric and magnetic properties. Beyond detailed knowledge of the dynamic properties of mention systems, the overall objective of this project is to increase knowledge and deeper understanding of the fundamental properties of materials, which in future will enable to create a new generation of nanodevices.