For nearly 60 years since its discovery in 1911 all known superconducting materials could be described by conventional Bardeen-Cooper-Schrieffer (BCS) theory, according to which itinerant electrons form pairs due to an attractive interaction provided by phonons. However it had changed with the discovery of $CeCu_2Si_2$, and following it UBe_{13} and UPt_3, heavy-fermion unconventional superconductors with large Sommerfeld coefficient and strongly paramagnetic susceptibility. Since then, the heavy-fermion superconducting materials have captured special attention.

A very significant and extensively studied family containing many heavy-fermion superconductors is $A_nM_mIn_{3n+2m}$ (where M is a transition metal Co, Rh, Ir, Pd or Pt and A is Ce, U, Np or Pu). One of the important members of this family is a heavy-fermion superconductor $CePt_2In_7$, whose neptunium analog we will investigate in this project. The reason of such interest given to the members of this family lies in the opportunity to study the interplay between magnetism and superconductivity in these compounds. It is suggested, that the origin of the superconductivity in these systems is due to the magnetic spin-spin interactions. The grant proposal aims at understanding the basic principles that govern the magnetic material $NpPt_2In_7$. The main goal of the project will be the theoretical investigation of the electronic structure and magnetic character of a new antiferromagnetic intermetallic compound from the “127” group. $NpPt_2In_7$ is a newly discovered compound, a Np analog of a heavy-fermion superconductor $CePt_2In_7$.

The project is planned for two years. In that time we plan to perform the full theoretical analysis of the investigated system. Due to the essential role of electron correlations in neptunium-based materials, the standard theoretical methods are insufficient to determine the physical properties of such compounds. Therefore we will perform the analysis using advanced density functional theory (DFT) methods, including relativistic effects. We will determine the magnetic ground state of $NpPt_2In_7$, calculate the electronic density of states (DOS) of the compound, its band structure, and Fermi surface. Investigation of antiferromagnetic material $NpPt_2In_7$ will enable understanding of the nature of magnetism in this compound. Moreover, the replacement of rare earth Ce with heavier actinide element Np, without significant changes in the structure gives a significant opportunity to study the electronic correlations in materials from $A_nM_mIn_{3n+2}$m family. The results of theoretical calculations are essential to plan further experiments and may guide experimentalists in their work of searching new compounds with fascinating properties.