A quasicrystal is a condensed phase of matter showing a special kind of spatial arrangement of atoms. In contrast to classical crystals, they lack translational symmetry, however, patterns created by local clusters of atoms occur in an orderly manner. An excellent example of a quasicrystal used in teaching is the Fibonacci chain, composed of two types of segments, long (L) and short (S). It is created in an iterative way, where a short segment is replaced by a long segment in the next iteration and a long segment is replaced by a combination of a long and a short segment. The initial condition is the existence of a short segment. An example sequence is as follows: 1) S → 2) L → 3) LS → 4) LSL → 5) LSLLS → … . The sequence has a strict order of successive occurrences of long and short segments, but the distances between segments of the same type are different. Due to the presence of long-range order, quasicrystals, according to the new definition of the International Union of Crystallography from 1991, are crystals, but to distinguish them from classical periodic crystals, they are referred to as aperiodic crystals.

At present, we know many metallic quasicrystalline phases occurring mainly in aluminum and zinc alloys. An important group are icosahedral quasicrystals. They are quasicrystals that are aperiodic in every direction of the crystal space. For example, decagonal quasicrystals have a single direction in which the layers of atoms are arranged periodically. Icosahedral quasicrystals have attracted the attention of researchers because of the presence of this phase in alloys with rare earth elements, which are known for the presence of localized electronic states of the 4*f* subshell, responsible for their magnetic properties.

In 2021, the occurrence of long-range ferromagnetic ordering was discovered in the Au-Ga-(Gd, Tb) alloy, which became the motivation for our research. This was the culmination of 20 years of research into magnetism in quasicrystals, where the basic unit of structure is Tsai clusters. Our research is also focused on rare earth quasicrystals, but in the group of Bergman phases. The two groups couldn't be more different. Bergman phases show a concentration spectrum of rare earth atoms, from 5-11%, where the Tsai phases have a strictly defined concentration of ~14-15%. Such a variety of concentrations of magnetic atoms in the structure creates an opportunity to explore the impact of the distribution of rare-earth atoms onto the magnetism of these quasicrystals. The Bergman group, although attempts had been made to study its magnetic properties in the past, was abandoned in favor of the Tsai group because the atomic structure of the latter was known. The atomic structure of the Bergman phase was solved only in 2020 by a member of our project team. Armed with new knowledge, we decided to conduct research on magnetism in the group of Bergman quasicrystals on a largest scale ever before.

In particular, Zn-Mg-{Gd, Tb, Dy, Ho, Er, Tm, and Y} quasicrystals, for which the growth conditions are known, will be studied. After receiving the above phases, we will try to synthesize crystals with the remaining rare-earth atoms. We intend to conduct detailed structural studies of these quasicrystals to understand the atomic environment of the rare-earth atoms. This environment has an important influence on the spatial arrangement of magnetic moments, and thus getting to know it is necessary to understand the results of experimental research. As for magnetism, we will study both static and dynamic arrangements of moments. Neutrons will be necessary as electrically neutral but magnetically interacting particles. Thanks to neutron diffraction, we will be able to study the ordering of magnetic moments in the structure in a long-range way, by observing Bragg peaks, but also local correlations observable in diffuse scattering. Experimental methods will be supported by computer methods, in particular we will use the DFT to estimate the values of the parameters of the 4*f* electron exchange interaction. Such calculations are rarely performed for quasicrystals due to the lack of periodic symmetry. In our calculations, we will focus on a finite number of atomic clusters. Carrying out calculations for a few selected local configurations of atoms will allow to estimate the energy of the magnetic interaction and consequently will allow to simulate the magnetic ordering and dynamics of moments in the context of experimental results.

The research proposed in the project concerns a fundamental issue. Magnetic interactions are the basis of modern civilization. Quasicrystals are magnetic materials with the highest possible symmetry. This means that such materials should exhibit the very low coercive field expected in any AC device. Our research will reveal the nature of magnetic interactions in aperiodic crystal alloys, extending existing knowledge in this unique form of condensed matter.