Since the discovery and first studies of graphene, two-dimensional materials experience a continuing interest of researchers, due to their excellent physical properties allowing to develop novel optoelectronic devices. Up to now, several hundreds of two-dimensional materials have been synthesized and currently they are being introduced to the common use. In the last years, a new class of two-dimensional materials that are simultaneously semiconducting and magnetic, has been discovered. Their existence is surprising, since the stability of magnetic ordering in two dimensions was forbidden according to the early theories. Numerous experiments have invalidated this thesis, and two-dimensional magnetic semiconductors have opened new possibilities of applications in electro, opto- and spintronic devices. They can also be employed in synthetic layered heterostructures, consisting of two-dimensional materials with various properties. For these reasons, experimental and theoretical investigations of magnetic semiconductors are highly desirable.

The fundamental feature of magnetic materials, determining their physical properties, is the type of magnetic moments ordering in the crystal lattice. One of the experimental methods of its investigation is optical spectroscopy. The optical spectra of materials result from their electronic and excitonic structure. Previous experiments and theoretical calculations have indicated a strong impact of the magnetic ordering type on the optical spectra of two-dimensional materials. A deeper insight into this dependence can be gained from optical measurements in high external magnetic fields. Energetic shifts of excitonic lines in magnetooptical spectra are quantified by the so called excitonic g-factors and diamagnetic coefficients. Values of these parameters can be precisely determined from theoretical calculations and support the identification of magnetic ordering in the studied materials, as well as deepen the understanding of the structure and properties of excitonic complexes hosted by these materials.

This project is focused on comprehensive investigations of magnetooptical properties of selected two-dimensional magnetic semiconductors with the use of modern numerical methods of quantum physics. Calculations of g-factors and diamagnetic coefficients of individual charge carriers and excitonic complexes in compounds from the families of transition metal di-, tri-, tetrachalcogenides, metal chalcogenide halides and MA_2Z_4, as well as their layered heterostructures, are planned, with a study of their dependence on magnetic ordering type, magnetization axis orientation and representation of electronic correlations. Moreover, exciton binding energies and Bohr radii will be evaluated to additionally support the interpretation of experimental data.

The investigations will be conducted in the framework of Density Functional Theory and Bethe-Salpeter equation, which are precise tools of material properties computations. In particular, exciton g-factors will be calculated with the method that has recently been developed by the Principal Investigator, yielding excellent agreement with experimental results and currently commonly used in by theoretical researchers. Within the project, new computational tools will be developed and extended to allow automatization of calculations of the magnetooptical parameters in semiconducting materials.

The outcomes of the project will help in deeper understanding of physical properties of two-dimensional magnetic semiconductors and indicate new candidates for technological applications. Particularly, a result of the project will be a large set of magnetooptical parameters in a vast class of materials, essential for interpretation and planning of experimental studies in the near future. The developed numerical tools will be useful for a large community of theoretical physicists.