Since the discovery of graphene in 2004 – a one-atom thick hexagonal structure composed of carbon atoms – and its unusual properties, interest in two-dimensional systems has been continuously increasing. Transition metal dichalcogenide based materials, like molybdenum and tungsten compounds with sulfur, selenium and tellurium are particularly appealing. In the two-dimensional form they are semiconductors emitting light in the visible range, which enables their application in e.g. transistors, photovoltaic cells and optoelectronic devices. The symmetry of their structures and the presence of heavy metal atoms lead to the coupling of their optical and spin properties. This phenomenon provides great opportunities for the progress in optoelectronics, for example in the field of quantum computers.

The progress in synthesis techniques of these materials allowed to obtain the so called van der Waals structures, which contain two or more single atomic layers placed on top of each other – like Lego bricks. This enabled tuning the properties of materials in order to obtain the characteristics desirable for specific applications. Their understanding and utilization require experimental and theoretical studies. The latter have not been fully developed yet to quantitatively characterize and predict the properties of van der Waals structures.

One of the investigation methods of semiconductors properties is measuring their optical spectra in magnetic field. It gives an insight into e.g. the character of excitons – specific particles which are present in semiconductors and determine their optical properties. An external magnetic field changes the excitonic energy, which manifests itself in the shift of peaks in measured spectra and is described by so called g-factors. In two-dimensional materials these parameters reach unprecedented values, which stimulates current experimental and theoretical studies. Values of g-factors depend also on factors like strains, electric field, interlayer stacking and twist angle van der Waals structures. Understanding these dependencies is of fundamental importance for research of these materials and their technological applications.

The objective of this project is to investigate excitonic properties of van der Waals based on the following material families: orthorhombic monochalcogenides, hexagonal transition metal dichalcogenides and trichalcogenides, as well as recently developed MA_2Z_4 compounds. Calculations will be performed within Density Functional Theory – a quantum-mechanical method that allows to precisely determine the g-factors. Moreover, the effect of external factors: strains, hydrostatic pressure, electric field, and configurational factors: heterostructure composition, interlayer stacking and twist angle, will be studied. A new method of numerical investigations of hybrid excitons will be developed. Calculations results will support the quantitative interpretation of the experimental findings of international collaborators. They will also constitute a basis of g-factors engineering in a wide class of two-dimensional structures. Moreover, they might potentially allow to predict the properties of new, so far unexplored materials. The effects of this project will contribute to the fundamental materials research by means of theoretical and computational physics, which are essential to design new technologies and optoelectronic devices.