1. Research Project Objectives

The <u>aim</u> of the project is the experimental and theoretical studies of fundamental properties of advanced two dimensional (2D) materials, namely van der Waals heterostructures of group IV transition metal monochalcogenides (TMMC's), such as GeS, GeSe, SnS and SnSe. The monolayers, bilayers and a few layers structures of TMMC's constitute a new class of 2D semiconductors.

<u>The main objective</u> of submitted project are the pioneering advanced studies of physical properties of modern nanomaterials for anticipated applications reaching beyond solid state physics, into telecommunications, computing and material sciences. We are going to work out methods of elaboration of thin TMMC's layers (from a few down to a monolayer) and perform subsequent studies of their optical and electronic properties. We will focus our investigation on the impact of strong confinement and in plane anisotropy on excitons formed in these crystals, also subjected to magnetic fields. The <u>challenging</u> task of the project is the experimental determination of the energy level ordering of the exciton states in the monolayer and bilayer TMMC's, and verification theoretical <u>predictions/ hypothesis</u> that despite the strong binding such excitons can be interpreted in the frame of Mott-Wannier model. The additional <u>objective</u> of our research is demonstration that unique properties of 2D heterostructures of TMMC's, such as the tuning of the optical energy gap, robust excitons and the strong in plane anisotropy can be engineered and applied in novel optoelectronic devices.

2. Significance of the project

The first successful elaboration and the studies of monolayer graphene promptly bring on the interest to other 2D materials, such as transition metal mono- and dichalcogenides (TMMC's and TMDC's) hexagonal boron nitride, black phosphorus, to list a few. As other 2D materials TMMC's are expected to show systematical changes in structural, electronic and optical properties with the reduction of dimensionality. Additionally, due to the strong in-plane anisotropy these binary phosphorene analogues offer a new platform to the study many body effects in strictly 2D systems. TMMC's exhibit strong anisotropy in the optoelectronic properties. Moreover, due to unique electronic properties, they show potential for applications in optoelectronics, computing, telecommunication and energy conversion. Electronic, structural, and optical properties of TMMC's in the form from bulk down to monolayer have been an object of intensive theoretical studies. However, due to the difficulties in elaboration of thin TMMC's flakes from a few down to monolayer their experimental studies are still to be done.

3. Research Methodology

The project is closely related to the elaboration of thin TMMC's layers from a few down to a monolayer. We will make use of the experience from our previous elaboration of monolayer TMDC's. The research planned within this project involves both experiments (mainly optical spectroscopy) and theory (including large-scale numerical calculations). The electronic and optoelectronic properties of the studied heterostructures, such as optical and quasiparticle energy gaps, binding energy of excitons, polarization of absorbed and emission light, phonon energies, etc. will be determined in combined polarization resolved reflectivity (pseudo absorption) photoluminescence, photoluminescence excitation and Raman scattering measurements in which our group has a considerable experience. Most experiments will be done in our laboratory using existing infrastructure and the new systems funded by this project. Our group is well equipped in advanced apparatuses for the elaboration and study of 2D heterostructures. Some experiments requiring particular equipment unavailable in Wroclaw will be done outside, in collaboration with our Polish or foreign partners.

Experimental studies will be aided by theoretical analysis and numerical calculations. One particle spectra will be analysed in standard way, while in the study of exciton complexes we will implement methods of exact diagonalization of the interaction Hamiltonian matrix in the configuration basis for a finite number of particles in which a group has a considerable experience.

4. Research project impact

The study of optical and electronic properties of van der Walls heterostructures of group IV transition metal monochalcogenides planned in the project will enlarge fundamental knowledge of the physics of strictly 2D systems. The results of our investigation can have further potential impact on the other scientific disciplines and can be applied in novel electronic devices. Also important will be the involvement of students in the scientific research on today's forefront of elaboration and studies of novel materials.