The idea of quantum information processing and quantum computers is undoubtedly one of the biggest and, at the same time, the most fascinating scientific challenges, that may lead to the next unprecedented technological revolution in 21st century. Unlike traditional computers, where each value representing the processed data is encoded as a combination of zero and one, which corresponds to two distinguishable voltage values on the transistors, in quantum computers the data is represented by the quantum state of the system constituting the quantum microprocessor. The basic building blocks of quantum computers are quantum logic gates called qubits, which can simultaneously have a value of zero, one, or any quantum superposition of these two states. The most enigmatic physical phenomenon, which is the foundation of quantum computing, is the so-called quantum entanglement. This phenomenon occurs, when groups of objects interact with one another in such way, that the quantum state of each individual object cannot be described independently but instead, a quantum state must be described for the system as a whole. Gaining access to the entangled quantum states is the key to exploiting the exponentially large computational power of quantum systems. Nevertheless, entangled states are very sensitive to various decoherence sources. For this reason, the main challenge is to create a perfectly controlled environment where large entangled states can be generated and manipulated without interference. Such an environment can be a wide-bandgap semiconductor, in which the electron spin associated with a paramagnetic point defect represents the qubit quantum state. The prototype of such a defect is the nitrogen-vacancy center in diamond because of an individual addressability of its quantum states that can be initialized, coherently manipulated and read out with high fidelity at room temperature. Nevertheless, to design scalable quantum system based on qubits in diamond one need to introduce an array of many point defects, such as NV, into the diamond lattice in a controllable manner, which is a great challenge for the existing technologies. Therefore, the discovery of analogous defects and their engineering into the technologically matured host crystal should open up new perspectives in scalable quantum technologies.

Inspired by progress in diamond-based quantum information processing and the preliminary results for III-V nitrides, I am going to investigate various point defects and their complexes in bulk and two-dimensional AlN and GaN crystals. The main goal of the proposed project is to identify novel point defects in AlN and GaN for nanophotonic and quantum information processing applications, which can be successfully engineered in the host crystal. To achieve this goal, I am going to use the-state-of-the-art computational quantum mechanical approaches (such as hybrid density functional theory, time-dependent density functional theory, many-body perturbation theory GW), group theory, and computational thermodynamic tools. The expected results of the project are following:

- An extended database including formation and ionization energies, orbital energies and characters, optical signatures (excitation energies and ZPLs), IR and Raman signatures (quasilocal vibrational modes), hyperfine structures (A-tensors), zero-field splitting (D-tensors) associated with various carefully selected point defects and their complexes in 2D and 3D AlN and GaN structures
- A detailed theory on the potential optical spin-polarization cycles and possible control protocols of the plausible candidates for quantum information processing applications. Based on group theory considerations and high-quality numerical data, I am going to derive the effective Hamiltonians using symmetry adaptive basis sets for spin-spin coupling, spin-orbit coupling, electron-phonon coupling and piezoelectric effect as well as provide theoretical description of possible radiative and nonradiative transitions associated with these point defects
- Thermodynamic defect phase diagrams to predict the stability of the selected point defects, and to mediate a successful defect engineering

I am convinced that the results obtained within this project will broaden the knowledge about quantum behavior of point defects and their complexes in bulk and two-dimensional AlN and GaN crystals as well as will have a strong impact on the development of nanophotonics and quantum information processing. The identification of attractive candidates for quantum bits in AlN or GaN combined with their precise engineering in the host's lattice should allow us to create high-quality scalable quantum systems.