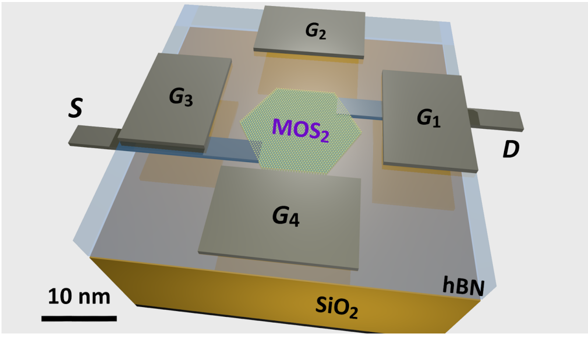
Realistic modeling of quantum nanodevices based on modern 2D materials



Research on physical realization of the quantum computer concept has sped up considerably in the last few years. Achieving quantum supremacy, i.e. the ability of quantum computing devices to solve problems that classical supercomputers practically cannot solve, by specialists from Google in their widely commented experiment, is an important step in the development of quantum computers. However, the implementation they propose, i.e. superconducting qubits, is burdened with a short coherence time (limiting the qubits' lifetime) and low gates fidelity. Low fidelity means that to build a single useful logical qubit we need at least 100-1000 physical ones. Therefore, the scale of quantum computation experiments is still far behind the current level of classical computations and new materials and new architectures are constantly being sought to realize the dream of a fully functional and practically usable quantum computer.

The “Realistic modeling of quantum nanodevices based on modern 2D materials” project directly addresses the challenges in optimizing the structure and operation of quantum nanodevices, capable of implementing qubits (i.e. basic elements of quantum computers) in solid state. Taking advantage of recent global progress in atomically thin van der Waals (2D) materials, the project will develop tools that help to optimize the state-of-the-art quantum technology hardware with functionalities enabled by the quantum properties of 2D materials, including Transition Metal Dichalcogenides (TMDs) and bilayer graphene (BLG). The unique interplay between electron charge, spin, and valley degrees of freedom in these materials enables various intriguing possibilities to define qubits.

This project will seek to realistically model all of these unique properties of 2D materials and to exactly model the device characteristics. Such precise description helps to analyze the influence of these properties on qubits manipulation and allows for optimization of this process. We will show that by exact modeling of the devices via coupling the Poisson solver describing the device electrostatics and the Schrödinger solver for monolayers, it is possible to *quantitatively* model the behavior of individual qubits and multiqubit registers. The outcome of this project will be a set of software tools which will allow for the realistic simulation of proposed quantum computing platforms based on emergent 2D materials and their heterostructures. This in turn will assist in identifying promising next-generation quantum computing platforms and help designing future experiments.