Due to the continuous increase in the global energy demand and the effects of fossil fuel consumption on the global warming issues, the development of alternative, sustainable and renewable sources of energy becomes a matter of urgency. Currently, traditional fossil fuels (petroleum, coal, natural gas) account for more than 80% of the global energy. Preliminary estimations suggest that in this century we will run out of petroleum (40 years), natural gas (60 years), and in the next century coal (150 years).

Hydrogen can provide an efficient solution to these problems and is considered as an ideal alternative to the fossil fuels. This is owing to its high energy efficiency, environmental friendliness, and non-toxicity. The benefits to the global economy cannot be underestimated either. The key issue to public acceptance of hydrogen energy systems is free of risk, proficient, and reliable storage. The main obstacle of the hydrogen technology is related to the development of a method for the convenient and reliable storage of hydrogen as well as on-demand releasing of it. One of such promising methods concerns the idea of solid-state hydrogen storage systems, featuring high storage capacities, low cost, efficient handling and transportation, as well as safety.

The biggest challenge of the hydrogen technology is the development of specific materials for efficient hydrogen storage. In this context, two-dimensional (2D) materials with remarkable chemical stability and extremely high active surface area, which exhibit excellent performance for hydrogen storage applications, appear to be of particular interest.

The project aims to utilize the ultimate 2D material – silicene as a next-generation platform for solid-state hydrogen storage. Silicene, a one-atom-thick 2D material, is a silicon counterpart of well known graphene. Owing to its remarkable electronic and structural properties, silicene was mainly explored in the context of modern nanoelectronics, but is also a subject of interest in the field of efficient hydrogen storage. However, it requires some functionalization, i.e. modifications of its physico-chemical properties. In the present project, the functionalization will be carried out in two alternative ways: (i) by synthesizing various silicene structures on the substrate, and (ii) by decorating it by atoms of metallic chemical elements. This should improve the performance of silicene in the context of the hydrogen capacity and energetics, as well as promote other mechanisms of hydrogen storage.

The project aims to perform a comprehensive study combining state-of-the-art experimental and theoretical approaches with their strong mutual interaction at each stage of the work.

The goal of the project is to determine mechanisms and conditions responsible for efficient hydrogen storage in silicene-based systems. The novelty of the project relies on the successful synergetic combination of functionalized 2D materials with specific substrates into advanced hydrogen-storage-oriented material complexes. Its realization should result in better understanding of processes and phenomena governing the interaction of hydrogen with functionalized 2D materials, and provide important clues for designing and building efficient silicene-based hydrogen-storage platforms.