Aim of the project

The main goal of the project is to provide new knowledge allowing to determine the relationships between the spatial structure and the chemical composition of core@shell nano-photocatalysts and their optical properties, which determine the possibility of enhancing their photoactivity in chemical reactions induced by visible light via localized surface plasmon resonance (LSPR).

Research description

In the research methodology, we will apply the computational design of the morphologies and simulations of properties of the core@shell nano-photocatalyst. New numerical tools will be developed that will allow for parametric design of the spatial, model, and explicit representations of the structures of such nanoparticles, taking into account the variations in geometric features (dimensions and spatial distribution). For many different variants of the generated structures, simulations will be carried out using the finite difference in the time domain (FDTD) method, which will allow the determination of effective absorption/scattering cross-sections of the visible light wave, as well as near-field intensity maps. Simulations will also be carried out using the density functional theory (DFT) to describe the atomic scale characteristics of the NP/support interfaces, and to determine dielectric constants for FDTD simulations. The use of parametric, multi-variational, numerical design approach will allow to prediction the properties of nanomaterials with many morphologies with less effort and reduce the number of time- and cost-consuming experiments.

Reasons for undertaking the research topic

Due to the growing energy demand, combined with the gradual depletion of fossil fuels and air pollution, there is a clear trend of searching for efficient alternatives for the utilization of non-renewable resources in energy production processes. One of the most intensively exploited topics by the research community is the use of solar energy as the driving force of chemical reactions. A process of particular industrial and economic importance is hydrogen production as the ‘fuel of the future’. The full potential of solar energy is possible by applying appropriate photocatalysts in the form of nanoparticles active in this range of the radiation spectrum. This activity is determined both by the appropriately selected chemical composition as well as by the spatial structure (morphology) of nanoparticles - the size and spatial organization of nanoparticles onto the core/shell surface. Appropriate shaping of the geometric features of composite nanoparticles allows for the intensification of physical phenomena occurring due to the interaction of nano-objects with an electromagnetic wave (e.g. the antenna effect). In recent years, the results obtained for core@shell nano-photocatalysts with SiO_2 core decorated with Pt nanoparticles, which were additionally immersed in a TiO_2 shell, were presented. Thus, a new model of light absorption was given, and the possibility of modulating the absorption peak of Pt nanoparticles in the visible range by adjusting their dielectric environment instead of changing their size. The absorption of light scattered by Pt nanoparticles in the near-field at the dielectric surface of the spherical SiO_2 core is intensified by plasmon resonance (LSPR), and the particles show distinct absorption peaks in a broader range of the visible light spectrum achieving significantly enhanced photocatalytic activity toward redox reactions. This discovery opens a promising path for using metallic (plasmonic) nanoparticles as the visible light photons’ absorbers in solar energy conversion processes.

Expected results

The execution of the project will provide comprehensive knowledge in the field of understanding the relationships between the morphology and the chemical composition of core@shell nano-photocatalysts and their optical properties, determining their performance in chemical reactions induced by visible light. Dedicated numerical tools will be created that will allow the design of nano-photocatalysts, taking explicitly into account sophisticated variations in morphology at the level of their spatial structure. Due to this, we will be able to scrutinize the influence of structural parameters of the investigated nanoparticles on the intensification of LSPR and tuning of the optical properties that determine their photoactivity. It is assumed that, on the basis of the numerical analyzes, a set of guidelines for successful design will be created, and the optimal variant(s) of the nano photocatalyst will be selected, which will be able to be synthesized and characterized experimentally in further work.