Mechanism of quantum dots excitation in photocatalytic reaction

Environmental pollution and the energy crisis have become two major problems for human society and can seriously threaten the quality of life. Semiconductor mediated photocatalysis has been accorded a great significance in recent times due to its potential to mineralize a wide range of organic pollutants at ambient temperature and pressures into harmless substances, to produce hydrogen in photocatalytic water splitting process, to produce hydrocarbon in CO_2 photoconversion (artificial photosynthesis), for inactivation of microorganisms as well as to apply in dye-sensitized solar cells.

Among semiconducting materials, zero-dimensional materials such as quantum dots have attracted recently the most attention. Quantum dots contain usually from 200 to 10,000 atoms (usually 2-10 nm) and due to high surface-to-volume ratio, they show unique features comparing to other nanomaterials.

One of the key problems in the application of nanomaterials in environmental protections as well as in solar to chemical energy conversion is the problem to obtain materials active in the presence of visible light, which constitute more of solar spectrum reaching the earth's surface. Thus, one of the observed trends is the usage of nanomaterials in size of quantum dots in environmental protection and energy conversion applications.

Thus, to enhance stability, utilization of visible light and to increase efficiency of photocatalytic processes, novel materials based on multilayer quantum dots, doped quantum dots and quantum dots modified by carbon species have been proposed in this project. Moreover, investigation of excitation mechanism depending on type of applying irradiation, as well as investigation of reaction mechanism occurring in the presence of novel materials, should allow for developing materials possessing higher activity in pollutants degradation, hydrogen generation in water splitting reaction and carbon dioxide conversion into useful hydrocarbons using solar irradiation.

Additionally, the project proposes the novel approach using chemoinformatics and computer modeling methods, which should allow in the future for modern design of new nanomaterials with enhanced functionality and to reduce the cost of experimental research.