Mendeleev 2024

XIII International Conference on Chemistry for Young Scientists

BOOK OF ABSTRACTS

St Petersburg University

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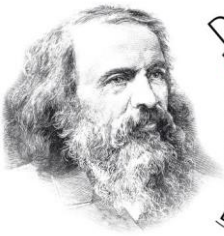

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Cr-DOPED SnO_2 NANOPARTICLES: INFLUENCE OF SYNTHESIS CONDITIONS AND STRUCTURAL PARAMETRES ON PHOTOCATALYC ACTIVITY

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Water purification becomes a main improvement tool of sanitarian and epidemiological state of the environment. However, the water pollution problem is increasing drastically due to active global urbanization processes and conventional methods faces serious problems due to large-scale production of hazardous organic pollutants. Nowadays the major entry route in the environment is the wastewater of various manufactories, such as textile production. In this regard, it is necessary to develop fast and eco-friendly utilization. Semiconductor photocatalysis using doped SnO_2 nanoparticles is a modern technique which has received tremendous attention as a cutting-edge approach for waste-free water purification.

Doping of SnO_2 with rutile-type crystal structure, tolerant to substitution, with 3d metals is a widespread way to improve the photocatalytic efficiency and also to provide additional functional properties, such as luminescence, in order to provide a monitoring of the photocatalyst stability and reusability. Among various 3d metals Cr^{3+} is the only affordable and profitable from an economic point of view dopant which can be used to obtain multifunctional photocatalyst. However, aspects concerning regulation of photocatalytic properties in order to improve the degradation efficiency are still unresolved. The aim of this research is to investigate the relationship “synthesis conditions, structural parameters, and photocatalytic properties” for Cr-doped SnO_2 nanoparticles (NPs).

Co-precipitation method and its combination with post-synthetical hydrothermal treatment (HTT) led to the synthesis of nanoparticles of spherical and cubic shape, respectively. Synthesis was performed using pH 3 and 7, dopant concentrations varied form 11 mol% and 33 mol%.

As-prepared NPs were characterized by a complex of physico-chemical methods. According to XRD data, all samples represent the rutile-type structure, no additional phases were observed. Successful doping was confirmed by changes in lattice parameters, hydrothermal treatment led to an increase in crystallinity. According to HR-TEM and SAED data, 4 nm spherical and cubic nanoparticles with polycrystalline structure can be observed, while EDX results indicate a uniform distribution of dopant in the structure.

The band gap energy, including direct and indirect transitions, was analyzed by absorption spectroscopy, which was confirmed by quantum-chemical calculations using our original approach. The amount of defects and oxygen vacancies was determined using XPS and Raman spectroscopy, respectively. It was shown that hydrothermal treatment reduces the amount of defects. An original computational approach was used to determine the optimal dopant position of substitution based on quantum-chemical calculations using DFT method, considering our dopant concentrations. It was found that the dopant position and the composition of the reaction medium affect the morphological parameters of nanoparticles. Moreover, various dopant concentrations allow us to regulate amount of oxygen vacancies and defects.

A comprehensive study of photocatalytic properties on the example of methylene blue (MB) under UV-light was performed according to our developed protocol, which includes several stages: study of kinetics of photodegradation and dark adsorption, investigation of surface composition by FTIR method, quantum chemical calculations of the interaction energy between NPs surface and pollutant molecule, study of mass spectra of by-products, investigation of active species by scavenger test and reusability properties by stability test.

Optimal sample with 11 mol% of dopant, obtained at pH 3, demonstrate 88% of MB decomposition in 90 minutes. It was shown that the efficiency of photocatalysis is affected by the expression of the “dye molecule- photocatalyst surface” interaction.

Thus, multifunctional NPs Cr-doped SnO_2 can be used as promising material for recyclable and effective wastewater treatment.

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