



# Mendeleev 2024

XIII International Conference on Chemistry  
for Young Scientists

# BOOK OF ABSTRACTS



St Petersburg  
University

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**XIII International Conference on Chemistry  
for Young Scientists “MENDELEEV 2024”**

St Petersburg, Russia  
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2024

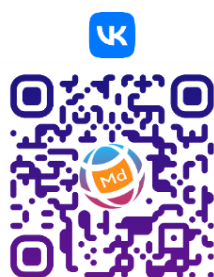
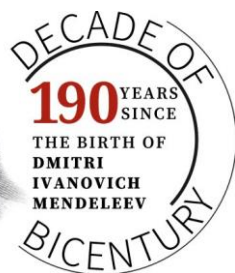
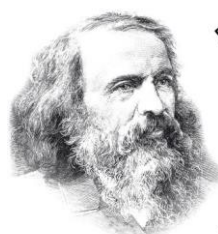
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# ENHANCING ANTIBIOTIC REMOVAL FROM WASTEWATER USING TIN DIOXIDE NANOPARTICLES OF VARIOUS SHAPE: INVESTIGATING THE IMPACT OF STRUCTURAL PARAMETERS ON PHOTOCATALYSIS

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Currently, water pollution by cyclic organic compounds (COCs) such as dyes and antibiotics poses a significant environmental threat. Antibiotics enter wastewater through various technological processes and adversely affect the ecological state of water resources, since many of them are toxic and mutagenic. Additionally, without proper treatment, sulfonamides can persist in the environment for extended periods due to their stability, exacerbating their harmful impact.

Cost-effectiveness, environmental friendliness, and the simplicity of implementation are crucial factors for effective water purification. In this context, the photodegradation of cyclic organic compounds (COCs) using wide band gap semiconductor nanoparticles (NPs) is gaining traction. Photocatalysis involves the accelerated degradation of complex COCs facilitated by reactive oxygen species generated in the aqueous medium when light interacts with the surface of wide band gap semiconductor nanoparticles.

Despite the extensive understanding of the photocatalysis process, achieving optimal efficiency in practical applications requires identifying the specific factors and material characteristics that influence this process. However, the existing literature on this topic is limited. Semiconductor particles are characterized by a wide range of parameters that affect their properties. To determine the key factors influencing photocatalytic activity, it is sensible to begin by studying nanoparticles with similar morphology (i.e., the same size and shape).

Among the numerous semiconductor materials that demonstrate significant activity under UV radiation, tin dioxide  $\text{SnO}_2$  stands out due to its rutile-type structure, n-type semiconductor properties, and a bandgap energy of 3.6 eV. This work focuses on developing an approach to regulate the structural parameters of nanoparticles and exploring their relationship with photocatalytic activity.

Spherical NPs were synthesized by co-precipitation method. The synthesis temperature and reaction media composition were varied to change the rate of NPs formation. All samples were characterized by physico-chemical methods in a combination with quantum chemical calculations.

The organic dye Methylene Blue (MB) solution was used as a model system to study the kinetics of photodegradation under UV radiation. The optimal sample demonstrated 95% MB decomposition in 7 minutes. Consequently, this sample, exhibiting the best photocatalytic efficiency, was then used to test the photodegradation of a widely used sulfonamide antibiotic. The study revealed that a mixture of sulfonamides degrades less efficiently than individual antibiotics. However, more than 90% of all components in the mixture degraded within 35 minutes. It was shown that the rate of the photocatalysis process is determined by the energetic benefit of the interaction between antibiotics and the photocatalyst surface.

Initial spherical blocks with various amounts of oxygen vacancies and defects were used for post-synthetic treatment under hydrothermal conditions (HTT) and investigated via oriented attachment (OA) mechanism. Consequently, the size of the resulting rod-shaped particles was determined by the favorable interaction of different numbers of initial blocks, as evidenced by the decrease in lattice parameters. It was demonstrated, that the surface composition affects the shielding capabilities of the reaction medium components. The optimal sample demonstrate 75% degradation of MB after 7 min.

In summary, the amounts of oxygen vacancies ( $V_o$ ) and structural defects (D) were calculated using our original approach based on XPS and Raman spectroscopy data. The effect of the  $V_o/D$  ratio on the photocatalytic activity of the  $\text{SnO}_2$  samples was established for the first time. The results showed that samples with a higher number of vacancies and fewer defects exhibited improved photocatalytic efficiency.

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