Mendeleev 2024

XIII International Conference on Chemistry for Young Scientists

BOOK OF ABSTRACTS

St Petersburg University

BOOK OF ABSTRACTS

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

St Petersburg, Russia
September 2-6,
2024

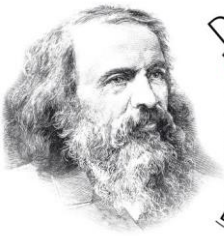
XIII International Conference on Chemistry for Young Scientists “MENDELEEV 2024”. St Petersburg. September 2–6, 2024. Book of abstracts.— St Petersburg.: VVM Publishing LLC, 2024.— 822 p.

ISBN 978-5-9651-1584-6

Book of abstracts contains theses of plenary, keynote, oral and poster presentations which were presented on **Mendeleev 2024**, the XIII International Conference on Chemistry for Young Scientists. The Mendeleev 2024 Conference hold in Saint Petersburg (September 2–6, 2024).

Abstracts are presented in the author's edition with minimal technical corrections.

DEDICATED TO



DECADE OF BICENTURY
190 YEARS SINCE THE BIRTH OF DMITRI IVANOVICH MENDELEEV

300 years Russian Academy of Sciences

300 YEARS of SPbU

@mendeleev.spbu

@Mendeleev_spbu

CONTENTS

THE CONTROL OF ZnO ORIENTED ATTACHMENT PROCESSES AS A TOOL FOR REGULATING ITS PHOTOCATALYTIC ACTIVITY

Meshina K.I.[1], Barabanov N.M.[1], Tkachenko D.S.[1], Bobrysheva N.P.[1], Osmolovsky M.G.[1], Voznesensky M.A.[1], Osmolovskaya O.M.[1]

[1] St. Petersburg State University, St. Petersburg, Russia
Student, undergraduate degree
kmeshina040301@gmail.com

Due to its antibacterial properties and non-toxicity, zinc oxide is engaged in the cosmetic industry (foundation creams, sunscreens) and medicine. Besides, a new urgent task is the use of zinc oxide as a photocatalyst for the decomposition of cyclic organic compounds that polluting wastewaters. Being a semiconductor, ZnO can be used for photodegradation of molecules, but there is a problem of creating an effective catalyst.

To solve this issue, it is worth referring to the fact that a feature of zinc oxide is the rapid course of the process of oriented attachment (OA) during synthesis. This topic has hardly been studied and opens up a lot of possibilities for regulating the structural and functional properties of ZnO.

In this work, based on our understanding of the OA process, counterions were used in the synthesis of ZnO nanoparticles, since this is the most easily adjustable parameter in the control of OA. Sulfate anion and nitrate anion were utilized as counterions. It is worth noting that there is a certain minimum in the form of structural blocks (hereinafter referred to as blocks), which are able to assemble in different ways into larger structures (nanorods, plates, flowers, etc.). In addition, during the synthesis, the holding time of the reaction mixture (0 and 90 min) and the order of reagents injection (SEQ – separately and SIM – simultaneously) were varied. The obtained samples were characterized by XRD, FTIR, SEM, SSA, XPS, Raman spectra, absorption and reflection spectra.

It was found out that the use of sulfate anions as counterions leads to the appearance of an additional phase of zinc hydroxide, therefore, zinc oxide nanoparticles obtained in cases of nitrate application were used for subsequent studies. The characterization also showed the presence of defects and oxygen vacancies in the ZnO structure.

Quantum chemical calculation methods were used to calculate the band structure of the samples, the interaction of the blocks with each other and the interaction of the surface of the blocks with ions present in the reaction mixture. Calculations revealed that the band gap energy corresponds to that obtained experimentally by constructing absorption spectra in Tauc plot. Moreover, it has been demonstrated that the most effective interaction is between blocks which surfaces are expressed by faces (0 0 1), while other faces (1 0 0) are “closed” to interaction because of adsorbed ions.

It is noteworthy, the OA process depends on which blocks are present in the reaction medium. In order to change the blocks and their varying connections, two procedures SIM and SEQ were used. Additionally, data analysis showed that holding the reaction medium for 90 min practically does not change the structural parameters of nanoparticles, which leads to the conclusion that the processes of block formation occurs directly while gaining the particles. The SEM data show the formation of grouped nanorods and flower-like structures using zinc sulfate. As for the use of the nitrate anion as a counterion, the formation of flowery clusters of nanoparticles in the case of the SIM procedure and nanoplates of the SEQ procedure was observed.

Photocatalytic activity was screened for four samples: ZnO particles were kept for 30, 60 and 90 minutes in a methylene blue (MB) dye solution, considered as a model of wasterwater, under the visible light radiation. The optimal sample turned out to be the one that was synthesized by the SEQ procedure using nitrate ions. The high efficiency of photodegradation is explained by the fact that this sample has a more accessible face (0 0 1) due to the assembly of blocks, which decomposes MB better under these conditions, which was also confirmed by quantum chemical calculations in our previous works.

Thus, the control of the process of oriented attachment makes it possible to regulate not only the morphological, but also the photocatalytic properties of ZnO nanoparticles.

Acknowledgements

This work was supported by the Russian Science Foundation (project No 23-23-00220). The research was carried out on the basis of the St. Petersburg State University Research Park, including the resource centers “RDMI”, “MASV”, “OLMIV”, “VC”, “Cryogenic Department”, “MRCNT”.