

BRIEF REVIEW

by Prof. PhD Antoaneta Borissova Trendafilova, Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences of the Doctoral Thesis presented for awarding the degree “**Doctor of sciences**” in the field of higher education: 4. "Natural Sciences, Mathematics and Informatics"; professional field: 4.2. "Chemical Sciences"; scientific specialty: "Organic chemistry"

Author: Prof. PhD Margarita Dimitrova Popova, Institute of Organic Chemistry with Centre for Photochemistry, BAS (IOCCP-BAS)

Topic: Novel approaches in the preparation of nanoporous materials with applications as catalysts or drug carriers

1. General description of the presented materials

The documents presented by Prof. Margarita Popova with respect to the thesis defence procedure are in accordance with the Regulations for the Development of the Academic Staff of the Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences (IOCCP – BAS), and meet the criteria of the Institute for obtaining the degree of “Doctor of Sciences”. Prof. Margarita Popova has provided a Doctoral thesis in English, Abstracts in Bulgarian and English, 28 publications not included in the PhD thesis, as well as a list of 678 citations of these publications.

Prof. Margarita Popova graduated from HICT-Sofia (now UCTM) in 1989 with a qualification „chemical engineer” in the specialty “Technology for organic synthesis and fuels”. In the period 1989 – 1991, she worked as a technologist – new productions in PLAMA-Pleven. She entered IOCCP-BAS in 1991, where she successfully defended her PhD dissertation in 1998. Over the years she has successively held the positions of specialist chemist, research assistant III, II and I degree. She was habilitated as an Associate Professor in 2011 in IOCCP-BAS. After winning a competition in 2017, she occupied the academic position of “Professor” in IOCCP-BAS. In the period 2012 – 2021, she held the position of Scientific Secretary of IOCCP. 1 She was elected Scientific Secretary of BAS in the field of „Nanosciences, new materials and technologies“ in 2021. So far, the scientific results of Prof. M. Popova are the subject of 110 articles published in renowned scientific journals, which are cited more than 1400 times. H-index is 22. Prof. M. Popova has been the leader of 5 projects, financed by NSF, of 4 bilateral projects, the Bulgarian representative in the Management committee of 3 COST Actions and participant in numerous research projects. Prof. M. Popova is a coordinator for IOCCP at the Centre for Excellence "Mechatronics and Clean Technologies" under the operational program "Science and Education for Smart Growth", a coordinator for IOCCP and a member of the Executive Board of NSP "Low-Carbon Energy for Transport and Domestic Use" EPLUS).

2. Relevance of the topic

The research presented in the dissertation is dedicated to the production of nanoporous materials with application in two important areas for human health: as catalysts for purification of the air from volatile organic compounds (VOCs) and as drug delivery substances. A number of EC directives in recent years have been aimed at limiting VOC emissions and protecting the

environment from them. As such, zeolites, modified mesoporous silicates or mesoporous metal oxides can be used, and the development of new procedures for the synthesis of nanomaterials with desired morphology, particle size and texture and for the modification of mesoporous silicates with metal / metal oxides or organic functional groups are an important prerequisite for their successful application in limiting and / or eliminating VOCs in the air.

The development of systems for controlled delivery and release of drugs based on mesoporous silicate materials, magnetic iron oxide / silicate mesoporous nanocomposites with different structure are very important areas in nanomedicine. The ability to surface functionalize and control the morphology and particle size of mesoporous silicate materials allows longer release of the drug substance and maintenance of its therapeutic concentration in the target functional area for a long period without side effects. All this defines the topic of the dissertation as very interesting and relevant.

3. Knowledge of the problem

The introduction to the dissertation summarizes in a very concise and clear way the achievements in both areas worldwide and shows an excellent knowledge of the issue. The Introduction contains an overview of nanomaterials and their application, methods for obtaining nanoporous materials and their role in the catalytic oxidation of VOCs, strategies for obtaining new drug delivery systems and the application of nanoporous materials in various biomedical fields. Guidelines for new research are outlined.

4. Research methodology

The methodological approaches used in the research in the dissertation work completely correspond to the set tasks. Both classical and up-to-date methods such as FT-IR and NMR spectroscopy in the field have been applied.

5. Characteristic and evaluation of dissertation thesis and contributions

The dissertation is written in English and contains 215 pages, which include 173 figures, 18 diagrams and 53 tables. In total 287 literature sources are cited. The topic of the dissertation fully corresponds to the scientific specialty. The goals and objectives are clearly stated. The "Results" section contains two main chapters: development of catalysts for complete oxidation of VOCs and development of drug delivery systems based on mesoporous silicate carriers. Mesoporous silicate carriers (MSM-41, SBA-15 and KIL-2, etc.) as mono- and two-component catalyst systems are mainly used. The role of the modification method and the specifics for the preparation of these catalysts, as well as their role in the process of complete oxidation of VOCs are clarified. A two-component catalytic system for the oxidation of VOCs and carbon dioxide based on cheap zeolites from coal ash obtained from the combustion of lignite coal has also been established. In the second direction, different procedures have been developed for the production of drug delivery systems such as amino-modified spherical MSM-41 and spherical SBA-15 with high adsorption capacity for ibuprofen and modified release of the loaded drug substance, mesoporous materials with carboxyl groups providing "soft" conditions and lower toxicity, verapamil delivery system based on bimodal mesoporous nanocomposites modified with $-SO_3H$ and $-COOH$ groups, etc. Drug delivery systems based on mesoporous silicates and polymers reacting to external stimuli have also been created for controlled and targeted delivery of anti-inflammatory drugs such as mesalazine, quercetin, etc. It has been found for the first time, that Ag-MCM-41, Ag-SBA-15 and AgY AgY materials loaded with sulfadiazine significantly improve its water solubility and antimicrobial properties. A procedure for loading sparingly soluble drug compounds by solid phase reaction has been proposed as a very effective method for stabilizing

their bioactive form. The scientific contributions are clearly formulated and have both scientific and applied character.

6. Assessment of the dissertation's publications and personal contribution

The results presented in the thesis are published in 28 scientific papers in international research journals from the first quartile in the respective field (Q1), and 1 of them is Q1, heading the field.. The number of the noticed citations of the publications included in the dissertation is 678. It is important to note that the publications related to the development of drug delivery systems based on modified mesoporous silicates and zeolites are the first on this topic by Bulgarian authors. The results of the dissertation were reported to 37 international scientific forums and were funded by 5 national and 3 international bilateral research projects, by the project for establishment of a Centre of Excellence „National Centre for Mechatronics and Clean Technologies“, National Scientific Program „Low-carbon energy for transport and domestic use“ (EPlus).

7. Abstract of dissertation

The abstract is in accordance with the dissertation and reflects the main results of the research. It also includes a list of publications included in the dissertation, as well as a list of projects that funded the research.

8. Personal impressions

I know Prof. M. Popova personally and I can say that she is an exceptional professional, a very good organizer and leader and a colleague who is always ready to share her experience and help, both professionally and personally.

CONCLUSION

The doctoral thesis contains substantial and significant original fundamental and applied scientific contributions, which meet all the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria, the Regulations for the implementation of the same Law and the corresponding Regulations of the IOCCP - BAS. The dissertation shows that Prof. M. Popova has in-depth theoretical knowledge and professional skills in the scientific specialty "Organic Chemistry" by demonstrating qualities and skills for conducting research in the interdisciplinary fields with original and significant scientific contributions.

Based on the above, I give my **positive assessment** of the research presented by the dissertation, results and scientific contributions and propose to the Honourable Scientific Jury to award the degree “**Doctor of Science**” to Prof. PhD Margarita Popova, in the professional field 4.2. "Chemical Sciences"; scientific specialty "Organic chemistry".

17.09. 2021 г.

Reviewer:

(Prof. Antoaneta Trendafilova, PhD)