

OPINION

submitted by Assoc. Prof. Dr. Ivanka Petrova Spasova, IGIC-BAS
on the Thesis for awarding the scientific degree "**Doctor of Science**"
in professional direction 4. 2 Chemical sciences, scientific specialty Organic chemistry
by Prof. Dr. Margarita Dimitrova Popova, IOCCP-BAS

Theme: ***NOVEL APPROACHES IN THE PREPARATION OF NANOPOROUS MATERIALS WITH APPLICATION AS CATALYSTS OR DRUG CARRIERS***

1. General presentation of the procedure and the candidate

The set of materials, submitted by Prof. Dr. Margarita Popova is in accordance with the requirements of ZRASRB, the Regulations for its Implementation of the Bulgarian Academy of Sciences and meets the criteria of IOCCP -BAS for obtaining the degree "Doctor of Science".

The candidate has submitted a Thesis in English, which reflects the results of 28 publications in specialized international journals with a high impact factors, which are not included in the dissertation for the educational and scientific degree "Doctor" and a list of independent citations of these publications.

Prof. Dr. Margarita Popova graduated from UCTM-Sofia in 1989 with a qualification of Chemical engineer, Master of Organic synthesis and fuels. From 1989 to 1991 she worked as a Technologist new productions in PLAMA-Pleven. In 1991 she started her work in IOCCP -BAS, where in 1998 she successfully defended her doctoral dissertation. Over the years she has successively taken the positions of chemist, assistant, chief assistant. In 2011 she was habilitated, and in 2017 she acquired the academic position of "Professor". From 2017 to 2021 she was Scientific secretary of IOCCP -BAS, and from 2021 she is Scientific Secretary of the Department of Nanosciences, New Materials and Technologies - BAS.

2. Relevance of the topic

The Thesis reflects a purposeful, comprehensive and systematic research directly related to the development of the very current field of nanotechnology and nanomaterials and their application in environmental protection processes and in medicine. It refers to finding new effective nanomaterials deposited on promising carriers for air purification processes and for drug delivery systems with targeted release. The research presented in the dissertation on the development of drug delivery systems based on modified mesoporous silicates and zeolites is pioneer for the Bulgarian science.

3. Knowledge of the problem

The candidate demonstrates excellent knowledge of the issue, which can be seen from a well-selected, concise and analytical literature review. Based on the unclear and missing

data on the problems in the air purification and on the delivery of medicinal products in the body, the purpose and tasks of the dissertation are clearly formulated.

4. Purpose, tasks and methodology of the dissertation

The aim of the dissertation is to present modern approaches for the development of new nanoscale materials with predetermined properties, favoring their application in two main areas: - as catalysts for processes related to air quality and as carriers of drugs, ensuring their controlled delivery in oral, dermal or parenteral systems. To achieve this goal, the development of catalysts for complete oxidation of volatile organic compounds (VOCs) and nanoporous materials for drug delivery systems based on monocomponent and bicomponent modified with metal oxides mesoporous silicates, zeolites and hybrid mesoporous silicate-polymers through new synthesis and modification procedures has been selected.

The methodological approaches used in the research are appropriately selected for the implementation of the tasks. A set of classical and template methods for the synthesis of nanomaterials are applied, mainly in the field of the soft chemistry. Active, selective and stable catalysts of mono and bicomponent oxides supported on mesoporous silicates and zeolites were synthesized. The carriers for the drug delivery systems are purposefully modified and functionalized to obtain materials with predetermined structural and surface properties. Magnetic composites have been created for the simultaneous delivery of anti-tumor and anti-inflammatory drugs. A set of various and complementary analytical methods and techniques were used to determine the physicochemical and adsorption-catalytic characteristics of the synthesized nanosystems - AAS, XRD, FTIR, TPR, TEM, Moessbauer spectroscopy, N₂-physisorption, AFM, solid-phase NMR, etc. The efficiency of the materials for complete oxidation of toluene as a model compound, as well as for static and dynamic adsorption of carbon dioxide was studied. In vitro release experiments on various drugs have been performed.

5. Characteristics and evaluation of the dissertation and contributions

The Thesis is structured according to the requirements and contains 215 pages, of which 13 pages "Introduction", combined with a concise overview, aim and tasks, 15 pages "Materials and methods", 156 pages "Results and discussion", 5 pages "Conclusions and contributions" and 6 pages "References", including 293 references. The Thesis is illustrated with 173 figures, 53 tables and 18 diagrams.

The literature review provides an overview of nanomaterials and their application, types of nanoporous materials and their preparation (special attention is paid to the silicate ones), complete catalytic oxidation of VOCs and strategies for obtaining new types of drug delivery systems. Based on the literature, the aim of the dissertation is derived and the tasks for its implementation are correctly selected.

In "Materials and Methods" an overview of the approaches for synthesis, the methods for characterization and the model testing on the studied nanomaterials is made.

The section "Results and discussion" accurately and precisely, with rich and informative illustration, reflects the results obtained in both areas of the Thesis.

The scientific contributions are original in the field of chemistry of nanomaterials and can be classified as a novelty for science and an extension of existing knowledge, with a potential for future practical application. They are divided into two groups. In the section "Development of catalysts for complete oxidation of volatile organic compounds", as a result of studying the relationship "synthesis-structure-properties" of monocomponent and bicomponent oxides deposited on mesoporous silicates and zeolites from coal ash, efficient catalysts for complete oxidation of VOC were obtained and optimized, as well as a two-component adsorption-catalytic system for oxidation of VOCs and adsorption of CO₂ has been developed. In the section "Drug delivery systems" was reported that for the first time in Bulgaria mesoporous silicates (appropriately modified and functionalized) for loading and stabilization of various drug substances with improved properties and targeted release were synthesized and used.

6. Evaluation of the publications and the personal contribution of the dissertation

The Thesis summarizes 28 scientific publications, and it is impressive that all of them are in quartile Q1 (Scopus/WoS), as one publication is in a journal, which is on the top of the respective ranking. The total impact factor of these publications is IF = 125.63, and the average impact factor of the publication is IF = 4.5. Prof. Popova is the first author in 10 publications, and in 18 publications she is the corresponding author, which is an unconditional proof for the leading contribution of the candidate in the ideas, planning and implementation of the research. The published scientific works have found a serious response in the world scientific literature in the field and are cited in 678 publications, which is a certificate of high quality and significant results in them. The results of the research on the topic are presented with 37 oral and poster reports at scientific conferences in Bulgaria and abroad. The research is funded by projects with the NSF, EU Operational Program, National Science Program and the inter-academic exchange between BAS and the Hungarian Academy of Sciences.

The scientometric indicators of the publications related to the Thesis of Prof. Dr. Margarita Popova significantly exceed the requirements of ZRASRB, BAS and IOCCP-BAS for awarding the scientific degree "Doctor of Science" in professional field 4.2. Chemical sciences.

7. Abstract

The abstract accurately and precisely reflects the main results presented in the dissertation.

CONCLUSION

The Thesis contains substantial and significant scientific and applied results, which represent an original contribution to science. The presented materials significantly exceed

all the requirements of ZRASRB and the Regulations for its Implementation, as well as the Regulations of IOCCP-BAS for awarding the scientific degree "Doctor of Science". The Thesis Prof. Dr. Margarita Popova demonstrates in-depth theoretical knowledge and professional skills for conducting targeted research. The high quality of the research, as well as the overall scientific activity of Prof. Popova as a distinguished scientist, give me reason to *convincingly give my positive assessment* of the Thesis, Abstract, Results and Contributions, and *to recommend to the esteemed Scientific jury to award the scientific degree "Doctor of Science"* to Prof. Dr. Margarita Popova in professional direction 4.2 Chemical Sciences (Organic Chemistry).

14. 09. 2021

Member of the Scientific jury:

(Assoc. Prof. Dr. Ivanka Spasova)