

PEER REVIEW

Opinion on PhD Thesis on the topic „Development of new metal oxides catalysts with application in alternative energy sources and ecology”

of Aleksandra Atanasova Mileva

submitted by Prof. Dr Alexander Eliyas, Institute of Catalysis - BAS

1. General presentation of the procedure and the PhD student

I was appointed as member of the Scientific Jury by an Order № ПД-09-328 dated 04.11.2020 issued by the Director of the Institute of Organic Chemistry with Center of Phytochemistry (IOCCP) based on Decision of the Scientific Council of IOCCP (Record of Proceedings №17 dated 29.10.2020) in accordance with Article 23 of the Regulations of IOCCP in regard to opening Procedure for the defense of PhD Thesis for acquiring the educational and scientific degree „PhD Chem. Sciences”. The PhD Thesis of Aleksandra Atanasova Mileva, regular form of education in the Laboratory „Organic Reactions on Microporous Materials”, professional area 4.2 „Chemical Sciences” in the field of Organic chemistry, specialty „Petrochemistry and Petrochemical synthesis”. The topic is „Development of new metal oxides catalysts with application in alternative energy sources and ecology”. The Jury had its first session at distance on 9.11.2020 and a decision was taken that I should prepare an opinion on the PhD Thesis with a deadline for submitting it until 20.01.2021 and the date of public defense should be 18.02.2021 at open session meeting.

The PhD student was enlisted for regular form of education in the specialty „Petrochemistry and Petrochemical synthesis” at IOCCP-BAS on 01.01.2016 and then she had interruption for maternity period 2017-2018. She had successful preliminary defence, followed by striking off the list as regular PhD student preserving the right for final defence and she was directed to a session of the colloquium for the defense.

2. Actuality of the research topic

This is a topic of exceptional actuality in present days in view of the growing consumption of fuels for internal combustion engines, both in the industry and in daily life, while at the same time there exists the opposite tendency of depletion of oil and gas deposits. This fact imposes the search for new energy sources, but these should be

such kind of resources, which should be in correspondence with the new more strict ecological requirements in view of protection of the environment. For this reason the focus of the PhD thesis is directed towards synthesis of new catalysts for reactions, in which one obtains chemical compounds i.e. the so called „hydrogen storage” compounds, possessing simultaneously the ability to store safely hydrogen and at the same time to be easily transferrable from place to place and to liberate hydrogen easily. An obvious example of such type of compound is methanol having high ratio H to C, whereupon it does not contain sulfur.

3. Knowledge of the problem

The evidence for having knowledge on the problem are the 742 literature references cited in the PhD thesis, which are commented on competently in the literature review in the introduction and the comments are specifically in connection with the aims formulated in the PhD thesis and the respective research tasks for achieving these aims. Moreover, one can also see from the 13 research publications, reporting the results of her PhD work, in which the PhD student is a co-author – this shows not only theoretical knowledge of the problem, but also impressive in scope and amount of data experimental research work. Therefore she has acquired practical skills and gained deep knowledge on the problem.

4. Methodology of the investigation

The methodology of the investigation represents an imposing complex of methods for synthesis (hydrothermal synthesis, urea assisted homogeneous hydrolysis), methods for physicochemical characterization such as XRD, BET method, FTIR spectroscopy – data on adsorption of pyridine on acidic active sites, Raman spectroscopy, XPS spectroscopy – formation of oxygen vacancies, TPR-TPG analysis, Boehm method of analysis, Moessbauer spectroscopy. Having kinetic profile of expertise I notice with satisfaction the level of the interpretation of kinetic data – catalytic activities, measured in two different catalytic reactions – oxidation of ethyl acetate and decomposition of methanol – conversion degree and selectivity and evaluation of apparent energy of activation.

5. Characteristics and estimation of the PhD Thesis and its contributions

As a whole the PhD thesis can be characterized as an impressive in bulk experimental research work, involving a large number of experimental methods, which without any doubt have contributed for the growth in scientific experience of Aleksandra Mileva. In my personal opinion the most valuable are the contributions involving the application of activated carbons from ecological point of view – utilization of waste material (peach stones, spent motor oil). On the other side there is a fundamental aspect of this contribution – elucidation of the mechanism of formation of the active sites occurring as a result of different methods of synthesis.

6. Evaluation of the publications and the personal contribution

The PhD student has a large number of publications – a total of 13 articles, whereupon she exceeds considerably the requirements with respect to a PhD thesis work. I would distinguish the publications in highly prestigious journals: Applied Surface Science, Applied Catalysis A: General, Journal of Environmental Chemical Engineering, Microporous and Mesoporous Materials. I notice with approval the support for the Bulgarian scientific journals - Bulgarian Chemical Communications, Journal of Chemical Technology and Metallurgy, Nanoscience and Nanotechnology.

I am convinced that her personal contribution consists in practical experimental activities, as well as in downloading the large number of literature sources – a total of 742 literature references, and also in assuming the essence in these sources, as well as in the application of some of their aspects in the course of the interpretation of her own experimental data and their computer processing. Of course during the interpretation she has obtained a powerful support and assistance by her scientific supervisor and scientific consultant. As far as the foreign authors are concerned and colleagues from IGIC-BAS and IC-BAS it is difficult to distinguish her personal contribution, but the important aspect here is the option to have access to scientific apparatus, which is missing in Bulgaria or in IOCCP.

7. Abstract of PhD Thesis

The Abstract of the PhD thesis in concise form represents the essence of the thesis comprising 20 figures and 22 tables are quite sufficient from the point of view of forming an opinion on the PhD thesis. The large number of citations observed shows

that her research work did not remain unnoticed, probably due to her good manner of presentations at scientific conferences.

8. Recommendations for future application of the PhD Thesis results

Being a catalyst specialist (recently in the field of photocatalysis) I would recommend the future application of the results, concerning the samples based on titanium dioxide on activated carbon, to be deposited as coatings and tested in the photocatalytic air purifier for closed premises, designed and constructed in IC-BAS.

CONCLUSION. The results, represented in the PhD Thesis of Aleksandra Mileva, are without any doubt significant contribution to the field of catalysis and respectively for the protection of the environment. The data throw some light on the structure, properties and activities of some new catalytic systems. An essential result of the carried out researchwork is the preparation of new and more active composite systems, which can find application in the ecology.

On the basis of the analysis given above about the investigations of the PhD Thesis I am convinced to recommend to the respectable members of the Scientific Jury to vote „YES” for awarding the scientific and educational degree „Philosophy Doctor in Chemical Sciences” to Aleksandra Mileva in view of the high level of the present PhD thesis, submitted to me for an opinion.

Sofia, 02.01.2021

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