

## ATTITUDE OF REVIEWER

by prof. Dr. Anton Naydenov

member of the scientific jury,

regarding the competition announced in State Journal no. 67 of 28. 07. 2020, for the awarding of the **academic position "Docent"** in the direction 4.2. Chemical Sciences (Chemical Kinetics and Catalysis), Institute of Catalysis (BAS)

**Candidate:** assistant professor d-r Radostina Dimitrova Palcheva, Institute of Catalysis (BAS).

Assistant professor d-r Radostina Palcheva was graduated for PhD thesis at Institute of Catalysis (BAS) in 2006 (PhD thesis "Sinergism between the component in NiW/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalysts for hydrodesulfuration), and in 2007 she occupied the position of assistant – professor at the Institute of Catalysis (BAS).

According to the minimal national and additional requirements of the Institute of Catalysis (BAS) in professional direction "4.2. Chemical sciences" (habilitation thesis – scientific in sources with reference and index numbers within the worldwide data bases (Web of Science and/or Scopus) of "group B", the total score regarding the publications (3 of them of Q1, 2 of Q2 and 1 of Q3) of d-r Radostina Palcheva is 130 points (at requirement of 100 points). Regarding the evaluating parameter 7 (scientific publications in sources with reference and index numbers within the worldwide data bases (Web of Science and/or Scopus, beyond the habilitation thesis) of "group G" are presented 14 publications (4 of them with Q1), the total score is 229 points (at requirement of 220 points).

The number of citations is 297. According to Scopus the H-index of d-r Radostina Palcheva is 12. Obviously, the candidate completes entirely the minimal national and additional requirements of the Institute of Catalysis (BAS) for the academic position "docent".

The scientific studies of d-r Radostina Palcheva are focused on the processes in production of ecologically clean fuels with low content of sulfur and nitrogen, more specifically on the hydrogenation processes as hydridesulfuration, hydrodenitrogenation and hydration of aromatic compounds.

Mo(W) – containing materials are used as catalysts, further promoted by nickel and cobalt with an interest directed to the factors defining the catalytic activity of Co(Ni)-Mo(W) catalysts in reactions of hydridesulfuration of thiophene (at atmospheric pressure) and 1-benzothiophene (higher reaction pressure).

Investigated are methods for preparation of catalysts and carriers, their chemical composition, thermal treatment, nature of the carrier, the influence of the modifying additives and complex forming compounds. Obtained are results regarding the catalytic activity of the catalysts by using of heteropolycompounds as model systems for preparation of mixed oxide catalysts. For additional objectiveness, the catalytic activity of the prepared catalysts is compared with the activity of industrial catalysts.

Prepared are active NiW catalysts, supported on TiO<sub>2</sub>, synthesized via hydrothermal method and the specific area of the prepared nanotubes is 285 m<sup>2</sup>/g. It is demonstrated that the application of Ti-NT as carrier significantly increases the catalytic activity in the reaction of HDS of thiophene, when compared with NiW/Al<sub>2</sub>O<sub>3</sub> and NiW/TiO<sub>2</sub> catalysts.

The results from X-ray photoelectron spectroscopy revealed, that after sulfation the catalyst contains significant amount of surface Ni sulfated species in close contact with W oxy-sulfides. It is suggested that within the predominant reduction media of most probably the surface Ti<sup>4+</sup> ions are reduced to Ti<sup>3+</sup> ions, which release electrons and additionally act as electron promoter to the W – sulfide phases.

Investigated are the possibilities for synthesis of heterogeneous catalysts by addition of metal oxide with basic character aiming to improve the interaction between the active phases and the carrier. The effect of ratio Zn to Al and the addition of SiO<sub>2</sub> to mixed Al-Zn oxides on the catalytic activity of NiMo catalyst in reaction of hydrodesulfuration of thiophene have been studied. The results from the X-ray diffraction show that Ni and Mo components are well dispersed on ZnAl<sub>2</sub>O<sub>4</sub>, obtained after calcination at 500 °C at low and middle Zn/Al ratio. At high Zn/Al ratio (0.57) an additional ZnO is formed which is interacting with Mo to form zinc molybdate.

It was shown that NiMo/Al–Zn<sub>x</sub> catalysts contain mainly Ni<sup>2+</sup> octahedral ions, MoO<sub>4</sub><sup>2-</sup> tetrahedral ions and Mo – polymer forms which amount and reducibility vary with the ratio Zn/Al. As a result from the additional modifying of Al-Zn oxides with silica, more surface MoO<sub>4</sub><sup>2-</sup> forms and NiMo/Zn–Al<sub>0.16</sub>–Si sample demonstrates higher conversion degree of thiophene within the temperature interval 280 - 400 °C. No increase in the catalytic activity is observed with the increased Zn/Al – ratio (0.24 and 0.60) and after addition of SiO<sub>2</sub> to the NiMo catalysts, which effect is explained by the formation of multilayered MoS<sub>2</sub> phases.

## Conclusion

The scientific studies of d-r Radostina Palcheva completely correspond to the theme of the announced competition for awarding the academic position "docent". The publishing activity after the habilitation, the citations of published results, participation and management of the projects and referee's activities completely cover the requirements of the Academic Staff Development Law and the Regulations on the Conditions and Procedure for Acquisition of Academic Degrees and the Occupation of Academic Posts at the Institute of Catalysis (BAS). Therefore, I convincingly recommend to the members of the Scientific Jury and to the Scientific Council of the Institute of catalysis (BAS) to award d-r Radostina Palcheva with the academic position "docent" under the direction "4.2. Chemical Sciences" (Chemical kinetics and catalysis).

Sofia, 10.11.2020.

Reviewer:

Prof. Dr. Anton Naydenov