

OPINION

on a competition for the academic position of "**Associate Professor**" in "Natural Sciences", professional field 4.2 "Chemical Sciences", scientific specialty "Solid state chemistry", announced in State gazette issue: 65, dated 28.07.2023 (page 48, ad #10)

with one candidate: **Veselina Tocheva Rangelova, Ph.D., Ch. Assistant**

Member of the scientific jury: Nikola Lyudmilov Drenchev, Ph.D., Assoc. Prof.

GROUNDs for the preparation of the opinion: Order No. ПД-38-526/01.09.2023 of the Rector of Sofia University "St. Kliment Ohridski" for the appointment of a scientific jury and decision of the scientific jury dated 04.10.2023 with Protocol No.1

1. General characteristics of the candidate's research and teaching activities

The research activity of Ch. Assistant Ph.D. Veselina Rangelova is mainly focused on obtaining, characterizing and researching of hydrogen sorption properties of Mg-Ni based alloys (amorphous and/or nanocrystalline), $\text{LaNi}_{5-x}\text{M}_x$ ($\text{M} = \text{Sn}, \text{Co}, \text{Al}$) and MmNi_5 in dependence on their chemical composition and microstructure. In addition, the research activity includes synthesis of "Metal-Organic Frameworks" (MOFs), characterization and investigation of their sorption properties with respect to CO_2 and H_2 .

The total number of scientific works of the candidate is **18**, of which **14** are referenced and indexed in Web of Science and/or Scopus. The remaining four articles are in non-refereed peer-reviewed journals or edited collective volumes. She is the author of a Monograph accepted for publication and the co-author of a textbook and a teaching aid. The total number of citations on Scopus is **176**, and the h-index of the candidate is **5**. Ch. Assistant Ph.D. Veselina Rangelova participated in **10** research projects, being the head of three of them. She has been the supervisor of **3** diploma theses and she has participated in **6** conferences.

The teaching activity of the candidate includes courses and practical classes in Inorganic chemical technologies for bachelor's majors (Chemistry FE and PE and Engineering Chemistry and Modern Materials FE) at Faculty of Chemistry and Pharmacy - SU, Department of "Applied Inorganic Chemistry". Ch. Assistant Ph.D. Veselina Rangelova has developed a course on "**Technologies for water, air and soil purification**" for the master's program "Ecochemistry".

2. Reference for the implementation of the minimum national requirements and the recommended requirements of the Faculty of Chemistry and Pharmacy - SU

Ch. Assistant Ph.D. Veselina Rangelova participates in the competition with a monograph accepted for publication, presented as a habilitation thesis and **12** articles outside the habilitation thesis. The points of "**Group of indicators C**" are **100** at required 100 points. The scientific papers for "**Group of indicators D**" are **12** (3 items - **Q1**, 4 items - **Q2** and 5 items -

Q3). Their total number of points is **230** at required **220** points. The candidate submitted a total of **174** citations under "**Group of Indicators E**" with a total number of points **348** at required **70** points. The collected points under "**Group of Indicators G**" are **155** at required **70** points.

3. Main scientific contributions

3.1 Main scientific contributions in the habilitation thesis (Monograph)

The reduction of greenhouse gases and the introduction of alternative energy sources to fossil fuels require the development and implementation of efficient technologies and materials for H₂ storage and CO₂ capture.

The monograph aims to review the achievements mainly in the field of hydrogen and carbon dioxide sorption in MOFs, to present the current progress and the main problems in this still developing research area, as well as to outline possible strategies for the improvement of the sorption characteristics of this new class of materials.

It gives some guidelines for improving the sorption characteristics of MOFs porous materials. The factors leading to an increase in the hydrogen storage capacity by strengthening its interaction with the active centers of MOFs, as well as the possibility of reversible gas sorption under "mild" conditions of their use have clarified. The conditions for achieving high selectivity in the separation of gases with importance in energy and ecology are also considered.

3.2. Major scientific contributions outside the habilitation thesis

The scientific works outside the habilitation work are grouped in two thematic fields: *(I)* Amorphous and crystalline materials with potential for hydrogen storage in the solid phase and *(II)* catalytic decomposition of ammonium perchlorate.

I would highlight the following contributions from the enumerated:

In paper **6**, LaNi₅-based alloys were investigated under hydrogenation/dehydrogenation, both gas-phase and electrochemically. The highest hydrogen absorption capacities were measured for the compositions LaNi_{4.3}Co_{0.4}Al_{0.3} (1.4 wt. % H₂) and LaNi_{4.8}Sn_{0.2} (>1.3%). A significant difference was found in the hydrogenation kinetics of all investigated alloys before and after activation (activation 5 cycles at 65°C, 40 atm. H₂). The activated alloys reach their maximum capacities in less than a minute, while the pure LaNi₅ alloy needs several minutes for fully hydrogenation. The discharge capacity of LaNi_{4.8}Sn_{0.2} decreases by only 10% for 60 charge/discharge cycles at a current density of 100 mA/g. A good agreement was also found between the hydrogen sorption kinetics of the alloys studied electrochemically and from the gas phase.

Paper **8** describes the results of electrochemical characterization of a series of AB₅-type alloys differing in composition, particle size, and crystallites as materials for negative electrodes in Ni-MH batteries. The influence of alloy composition and ball milling conditions on the morphology, microstructure, discharge capacity, and charge/discharge stability of the alloys has studied.

Regarding the electrochemical characteristics, it was found that the best effect was observed for the alloys milled for 5 hours under a hydrogen atmosphere.

The research in article 4 is focused on a series of metallic glasses (Zr-based Zr–Cu–Ni–Al–(Ag) obtained by rapid cooling from a melt. Their thermal characteristics (T_g , T_x , T_l) were determined by the DSC/DTA methods. It is found that increasing Zr content leads to lower T_x and ΔT_x . It was established that there are compositions with very little difference in melting temperatures but with significantly different intervals of supercooled melt, ΔT_x . Analysis of the results leads to the conclusion that the difference in the glass-forming ability of the studied alloys is mainly due to difficulties in the crystallization process, not due to the different stability of the melts.

Publication 1 presents the preparation of new mesoporous structures from aggregated CuO/Cu(OH)₂ nanoparticles. The studies carried out using TG and DSC showed that the new material exhibits excellent catalytic activity in the decomposition of ammonium perchlorate, approaching the best results for copper catalysts. It was found that the addition of 3 wt. % CuO/Cu(OH)₂ lowers the decomposition temperature of NH₄ClO₄ by 96 °C, decreases the activation energy from $86 \pm 4 \text{ kJ mol}^{-1}$ to $65.2 \pm 0.6 \text{ kJ mol}^{-1}$ and increases the total amount of released heat by 38.6 %.

4. Conclusion

The topics, on which Ch. Assistant Ph.D. Veselina Rangelova works are up-to-date and have both a scientific and an applied nature. The contributions are original and significant. The materials submitted for participation in the competition are in accordance with the theme of the announced contest. The scientometric data cover and exceed both the minimum requirements for holding the academic position "Associate Professor", according to the Law on the Development of the Academic Staff in the Republic of Bulgaria, as well as the additional requirements of the Faculty of Chemistry and Pharmacy - SU.

Based on the overall scientific research and teaching activity, I find it reasonable to suggest to the members of the Scientific Jury to give their positive assessment in the selection of Ch. Assistant Dh.D. Veselina Tocheva Rangelova for holding the academic position of "**Associate Professor**" in professional field 4.2 "Chemical sciences", scientific specialty "Solid state chemistry".

Date: 21.10.2023

Signature:.....

/Nikola Drenchev, Assoc. Prof. Ph.D/