

## REVIEW



in a competition for the academic position of "Professor" at the Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, announced in the State Gazette, issue 20 / 10.03.2020 in Professional field 4.2. Chemical sciences, scientific specialty "Physical Chemistry" with a sole candidate Associate Professor Dr. Dragomir Mladenov Tachev

**Member of the Scientific Jury:** Professor Dr. Nikolay Stoianov Boshkov, IPC-BAS

### 1. Brief biographical data about the candidate

Associate Professor Dr. Dragomir Mladenov Tachev was born on 08.07.1971. He completed his higher education at Sofia University "St. Kl. Ohridski", Faculty of Physics, in 1995, main subjects "Engineering Physics" and "Microelectronics". He entered IPC in 1996 as a Master of Physics and is still engaged in research - fundamental and applied scientific investigations. In 2005 he obtained the educational and scientific degree "PhD" in Physical Chemistry, and since 2009 he has been an Associate professor at IPC-BAS. He has completed two postdoctoral specializations in Germany, namely: at Humboldt University in Berlin, Faculty of Chemistry (2006-2007), and at the Helmholtz Center for Materials and Energy, Berlin (2007-2009). Associate Professor Tachev uses English and Russian languages at an excellent level, as well as German at a basic level.

### 2. Description and evaluation of the submitted materials

In the competition in which Mr. Tachev participated, he presented evidence for the following scientific production: published (mostly in appropriate specialized foreign journals) in total 49 articles with different numbers of co-authors, and the candidate is the first author in 14 of them - respectively under No. 2, 4, 5, 8, 9, 11, 13, 14, 16, 19, 20, 25, 26, 29 from the attached list of publications. Associate Professor Tachev is the second author in 9 articles (No. 6, 17, 22, 24, 32, 37, 40, 41, 45), and in another 9 articles (No. 1, 7, 15, 31, 34, 38, 42, 46, 49) – the third one. In two of the published issues (No. 19 and 25) he is the sole author. His "h-index" (without self-citations) is 13, i.e. definitely in the area of the so-called "Professor's h-index".

It is obvious from the submitted information that the candidate has scientific contacts with a wide team of Bulgarian and foreign co-authors given the complexity of the systems studied by him and the methods used. From his place in the author's teams, however, it can be concluded that Associate Professor Tachev has a significant contribution to the realizing of the experiments, as well as to the preparation of the published articles.

The list of publications shows that 23 issues (No. 1-3, 5, 6, 8-10, 12, 13, 18, 19, 22-24, 26-29, 32, 33, 39, 45) are published in journals from group Q1, 9 issues (No. 4, 25, 30, 34, 35, 37, 43, 47, 48) are in group Q2, 4 issues (No. 11, 38, 42, 44) - in group Q3, 3 pieces (No. 31, 40, 46) - in group Q4. In addition, Associate Professor Tachev participated as a co-author in one book chapter (No. 49) and in 9 other articles (No. 7, 14-17, 20, 21, 36, 41), which were published in full text in collections with reports at scientific forums (symposia, conferences, congresses and others with international and/or Bulgarian participation) or in journals without impact factor and/or SJR. The candidate has also attached a list of publications that do not repeat those submitted for the acquisition of educational and scientific degree "PhD" and for the academic position of "Associate Professor". Among the journals stand out a large number of prestigious publications in the field of Electrochemistry and Physical Chemistry such as: *Electrochemical and Solid-State Letters*, *Journal of Non-Crystalline Solids*, *Journal of The Electrochemical Society*, *Electrochimica Acta*, *Journal of Applied Crystallography*, *Surface and Coatings Technology* (all from group Q1) etc.

In my opinion, it is necessary to remind here that before his participation in the current competition, Associate Professor Tachev has defended a dissertation for educational and scientific degree "PhD" (2005) and also received his habilitation in 2009. Given the above, it is logical to accept to the list of publications of Associate Professor Tachev to be added his PhD Thesis and its Abstract, as in practice they are also scientific papers that have been the subject of review by highly qualified recognized specialists in this field. Based on this summary, it is clear that the professional qualification and high scientific erudition of the candidate are beyond doubt.

The list of participants in scientific forums shows that Mr. Tachev has participated as a co-author and independently with a total of 18 reports and presentations at 13 Bulgarian and international scientific events. Of the last 4 were held in Bulgaria and 9 abroad. In addition, he is a member of the teams of a total of 12 international projects. Of these, 11 are in line with international cooperation in the framework of inter-academic treaties and agreements - the EBR - and 1 is related to a topic proposed by NATO - „Science for Peace”. Associate Professor Tachev is also a participant in 9 national projects. From them, 2 projects are funded by programs with ministries and other departments, 2 - by Operational Programs, and 5 projects are funded by the Fund for Scientific Researches.

All submitted materials correspond to the topic of the competition, as the scientometric indicators fully meet and even exceed (in some cases over 8 times) the minimum requirements of IPC-BAS to the scientific activity of the candidates for obtaining a scientific degree and for holding academic positions (Tables 1 and 2 of Annex 1 to the Regulations on the Terms and Conditions for Acquisition of Scientific Degrees and for Occupying Academic Positions at IPC -BAS) as follows:

For "Professor": Group A - 50 points (required 50 points) and an additional 45 points are given for 2 publications in journals from the groups Q1 and Q2, respectively (established in NACID, Bulgaria); Group B - 182 points (required 100 points); Group D - 270 points (required 220 points); Group D - 976 points (required 120 points); Group E - 360 points (required 150 points).

### **3. General characteristics of the research and scientific-applied activity of the candidate**

In his previous activity, the candidate has carried out his scientific and applied research generally in two main areas:

- Area 1 - Investigation of the formation of the nanometric phase or characterization of the nanometric phase in different media and materials;

- Area 2 - Theory of small-angle X-ray scattering in multiphase systems.

In addition, Associate Professor Tachev has research in the field of X-ray computed tomography, related to the characterization of laser-treated and other materials. These investigations are classified in Area 3 - Other articles - from the Author's reference. The investigations are distinguished by systematicity, consistency and precision, as a complex approach is applied, in view of the content to be of interest both for the narrow specialists and for the interdisciplinary scientists. The numbering of the publications I use below is according to the list of all scientific papers so far, articles after No. 24 were published after the habilitation procedure of the candidate.

The main part of the publications of Associate Professor Tachev in Area 1 are related to the use of small-angle scattering of X-rays and neutrons, and the research was done on the available equipment in EU countries such as Germany and France. Thematically, they can be grouped into 5 main subgroups: (1) Primary crystallization of Ni in a subeutectic amorphous nickel-phosphorus alloy; (2) Metal nanoparticles in sodium-calcium glass; (3) Crystallization of  $Mn_xFe_{1-x}Fe_2O_4$  particles in oxide glass; (4) Nanoparticles in closed spaces; (5) Platinum based catalysts.

The articles from subgroup (1) are thematically homogeneous and refer to traditional for IPC topics on germination and crystal growth. Most of them [No. 2, 4-6, 11, 13, 14, 16, 17, 26] are related to a model system of a sub-eutectic nickel-phosphorus alloy. The methods of small-angle X-ray Scattering (SAXS) and neutrons (SANS) were used. They give with high statistical reliability the distributions of the individual components by size in the volume of solid and optically opaque media. The methods have been supplemented with the application of TEM to determine the most suitable shape of the particles for description, and a thermo-magnetic method for magnetic phase analysis has been developed. The data were compared with the data from differential scanning calorimetry and dilatometry [No. 2, 4, 6]. Studies on the precipitation of Ni in a Ni-P alloy were

performed with anomalous low-angle scattering (ASAXS) [No. 5, 8, 9, 11, 13]. The average composition of the particles and/or the dependence of their composition as a function of their size simultaneously with their size distribution and the composition of the main matrix are determined. It was found that the smallest particles released are not pure Ni, but contain a significant amount of it. The obtained data were compared with data from DSC [No. 26], showing that the kinetics of Ni separation in the matrix is consistent with the Kolmogorov-Avrami theory of universal crystallization.

Studies from the subgroup (2) include ex-situ and in-situ ASAXS and SAXS measurements of gold-doped sodium-calcium glass [No. 18, 20, 29]. It was found that no change in the composition with the particle size was observed. The data show that when annealing in the presence of X-rays, no so-called "Oswald maturation" can be observed, i.e. a process in which small particles dissolve and support the growth of large ones [No. 29]. Similar studies have been performed for a system of gold-silver alloy or bimetallic particles of the "core-shell" type [No. 23]. They have a spherical shape: the larger ones are of the "core-shell" type, with the core having a lower density.

The articles from subgroup (3) present data on the process of crystallization of spinel nanoparticles in oxide glass from the  $\text{SiO}_2/\text{Na}_2\text{O}/\text{Fe}_2\text{O}_3/\text{MnO}$  system [No. 30, 31, 32, 33, 34]. The main task is to determine the average size, the size distribution and the average composition of the nanoparticles in heat-treated samples, which is realized.

Subgroup (4) provides information on studies of the production in a closed hollow sphere (apoferritin macromolecule) of particles of  $\text{Fe}_3\text{O}_4\text{-}\gamma\text{Fe}_2\text{O}_3$  (magnetite/maghemite) [No. 21, 24], silver [No. 28] and some oxides in order to study the magnetic interactions between nanoparticles with strong magnetic properties, such as iron oxides. Two types of apoferritin were used and it was found that the difference in the distance between the protein molecules (i.e. between the magnetic crystals in them) in the crystalline and in the amorphous sample has a significant effect on the magnetic properties of the samples. The effect of copper on silicoaluminophosphate was also studied [No. 47] with a view to use it in practice.

The works from subgroup (5) are thematically related to the characterization of the properties of selected platinum-based catalysts placed on a powder support (the latter most often on a carbon basis) [No. 35].

Associate Professor Tachev's research in Area 2 includes the application of the SAXS method to multiphase multi-component systems - for example,  $\text{Al}_{89}\text{Ni}_6\text{La}_5$  alloy [No. 22] by introducing the so-called single phase scattering functions under vacuum or self-contained conditions.

The number of scientific publications summarized in Area 3 are related to the application of X-ray computer tomography [No. 37, 40, 41, 43, 45, 48, 49] the latter being applied to a laser-treated biocompatible polymer, subsequently coated with chemically deposited nickel or platinum [No. 37, 43] and for aluminum-ion battery [No. 45]. Included in that section are also some "more exotic" studies – for example rocks from Antarctica [No. 36], deciduous teeth [No. 41], mechanical stresses in metal glasses [No. 7].

#### **4. Basic scientific and scientific-applied contributions**

The main contributions of the candidate in the individual scientific areas of interest can be summarized to the following:

- The maximum entropy method has been shown to be sufficient to determine the distribution of spherical particles by their size using small-angle scattering. A method for simultaneous determination of the particle size and composition distribution in the precipitation of nickel in a nickel-phosphorus alloy has been developed, and the maximum entropy method has been modified with the possibility of simultaneous analysis of several scattering curves by several size distributions. The method for determining the average composition of the particles and/or the dependence of their composition as a function of their size simultaneously with the size distribution and the composition of the matrix containing them is indicated. The obtained experimental data confirm the non-classical Schmelzer's nucleation theory. In addition, it was found that the kinetics of nickel separation in the amorphous matrix is consistent with the Kolmogorov-Avrami theory.

- A complete quantitative characterization of the process of separation of gold particles in the sodium-calcium glass, i.e., depending on the annealing time, the change in the number of particles, the average size and their volume part are determined. For the first time, delayed or postponed Oswald maturation is observed in the same system under practically equal experimental conditions, explaining the reasons for this phenomenon. The latter can be used in an applied aspect in optoelectronics - with measured doses of radiation to manipulate the number and size of gold particles. In the study of bimetallic gold-silver particles, a new two-stage method for data analysis was created, allowing the calculation of the composition of the core and shell, the number of particles, as well as some features of the formation of the core.

- - When studying the crystallization of spinel particles in oxide glass, the size of the particles and their growth during heating were determined, as well as some features of the composition of the core during its formation. The obtained data are the main part of the PhD Thesis of Dr. Vikram Ragunvanshi, whose defense is significantly supported by the advice and guidance received from Associate Professor Tachev.

- The production of nanoparticles from  $\text{Fe}_3\text{O}_4\text{-}\gamma\text{Fe}_2\text{O}_3$  (magnetite/maghemite), some oxides and silver in the cavity of the apoferritin molecule is characterized, and the method can be used to control the particle size. The difference in the dispersion of apoferritin (monodisperse molecule) and the particles in its cavity (which are not monodisperse) was used. In the study of silicoaluminophosphate (catalyst) it was found that the copper added to it accumulates in certain places (on the surface, in the grid of the matrix or in the channels), which allows the variation of the characteristics by the method of production.

- The composition and size of carbon dust particles used as catalyst carriers have been established. These particles have a specific scattering curve at small angles. A major problem is the separation of the curve the carrier from that of the catalyst. It has been found that the composition of nickel particles deposited on a powdered carbon carrier is closer to that of NiO, Ni(OH)<sub>2</sub> and NiOOH than that of pure nickel. The method of determining the composition is an improved version of that of the silver-gold particles presented in [No. 23], using the ratios of the scattering contrasts, but not to the contrast at a selected energy, but to their average value.

- The candidate has two articles in which he is the sole author and where he presents his addition to the theory of small-angle X-ray scattering, related to multiphase multicomponent systems. A contribution is the introduction of single-phase scattering functions, representing its scattering in vacuum or independently, by deriving a generalized expression for the scattering invariance of a multicomponent multiphase sample. The theory allows the determination of the types of measurement schemes, their number and the minimum number of energies at which the measurements should be performed, and is not limited to ASAXS. This approach could also be applied in cases of neutron scattering.

- When examining an aluminum-ion battery, it was found that after its discharge the cathode does not return to its original state due to inhomogeneous expansion, the presence of mechanical stresses and structural changes.

In conclusion, on the basis of the submitted materials, I believe that a correct, precise and at a methodological level experimental work has been performed, with clearly defined and current topics, whose usefulness and significance for science and practice do not raise doubts.

## **5. Reflection of the scientific publications of the candidate in the Bulgarian and foreign literature**

Associate Professor Tachev provided information on a total of 488 citations on 33 of his articles published so far, most of which (472 issues) were taken from Scopus, and for one of the publications [No. 23] the available data are from Web of Science (16 issues). Article No. 18 has the

most citations (78 pieces), followed by No. 28 (66 pieces) and No. 1 (45 pieces), i.e. these three works have been cited a total of 189 times. It is also necessary to emphasize that in most of the quotations there is also a comment, which is an obvious proof of the indisputable interest in the articles themselves and the relevance of the research topic.

#### **6. Critical remarks and recommendations**

I have no critical remarks. However, I propose it appropriate to consider the possibility of filing some of the experimental data obtained as patent or utility applications.

#### **7. Personal impressions of the candidate**

I have known Associate Professor Tachev since his admission to IPC. In my opinion, he is an example of a correct and responsible colleague who is always ready to help when needed. I have excellent impressions of his scientific activity - his research was conducted competently and at a high professional level, and to a large extent they are a personal matter given his place in the author teams of publications and reports at scientific forums. The analysis and interpretation of the experimental data, as well as the conclusions and contributions are logical and well-founded. The number of citations found in the publications clearly confirms the importance and relevance of the current topic of the candidate.

### **CONCLUSION**

From the materials presented by Associate Professor Tachev I can conclude that in terms of quantity and quality his scientific output is completely sufficient, meets and even in some cases significantly exceeds the Minimum requirements of the recommended criteria for holding the academic position "Professor" at IPC-BAS. Tables 1 and 2 of Appendix 1 of the Regulations on the terms and conditions for acquiring scientific degrees and for holding academic positions in IPC-BAS). The candidate is a fully educated scientist whose high scientific qualification is indisputable. Based on all this, I strongly suggest to the Honored Scientific Jury to elect Associate Professor Dr. Dragomir Mladenov Tachev for "Professor" in Professional Field 4.2. Chemical sciences, scientific specialty "Physicochemistry".

Signature: ..

(Prof. Dr. N. Boshkov)

Sofia, 18.09.2020