

## STATEMENT

from Prof. DSc Venelin Enchev,  
Institute of General and Inorganic Chemistry - BAS  
of the materials submitted for the competition for the academic position of 'Associate Professor'  
Faculty of Chemistry and Pharmacy, Sofia University "St. Kl. Ohridski"  
in higher education professional field 4. Natural sciences, mathematics and computer science  
professional field: 4.2. Chemical Sciences (Theoretical chemistry)

In the competition for the academic position *associate professor* announced in the State Gazette, issue 52, July 31, 2019 by the Faculty of Chemistry and Pharmacy at Sofia University, Dr. **Miroslava Nedyalkova** is the only candidate. The set of materials submitted by the applicant in electronic form is in accordance with the Regulations for the development of the academic staff.

I do not personally know the candidate. My opinion is based only on the documents submitted.

Miroslava Nedyalkova graduated as a Master with a degree in Chemistry and Qualification Master's degree in Medical and Pharmacological Biophysicochemistry from the Faculty of Chemistry and Pharmacy at Sofia University in 2006. From 2007 to 2016, she is an Assistant Professor, and from 2017 until now she is a Principal Assistant Professor at the Department of Inorganic Chemistry at the same faculty. In March 2014, she defended a thesis in theoretical chemistry on *Computer Nanoparticle Research: Effects of Metal Ions, Solvent and Citric Acid*. The dissertation is defended at the University of Sofia, but seems to be in common with the University of Barcelona. Unfortunately, the dissertation author's abstract is not attached to the application documents. Her publishing activity has become very impressive since she became Assistant Professor in 2017: 6 articles in 2019, 5 articles in 2018 and 8 - in 2017, most of them in Q1 and Q2 quart magazines. She is a contributing author in 10 of these 19 articles, which definitely shows her leading role in them.

Dr. Miroslava Nedyalkova has applied a total of 31 scientific works, of which 29 publications, 1 book chapter and one monograph. A list of 34 participations in scientific conferences (no abstracts presented), 9 conference organizing committees, a guide of 5 and participation in 16 research projects and a guide of 1 graduate student (but no year specified) were reported.

The candidate participates in the competition with 15 articles and one monograph. Five of the articles are on indicator C instead of habilitation work, and ten on indicator D, outside habilitation work. The competition papers present a variety of studies and this may be the reason why scientific contributions are not to be summarized in one or more directions but to be presented separately for each article.

The articles included in the habilitation work (three with quartile Q1 and two with quartile Q2) used three different research approaches - with quantum-chemical methods, with molecular dynamics and cluster analysis. With *ab initio*, quantum-chemical methods have demonstrated the possibility of delocalization of the proton between two or three carboxylate groups at citric acid conformers, as well as intramolecular transfer of the proton through low energy barriers. Molecular dynamics has revealed the mechanism of tearing a thin toluene emulsion film in contact with the aqueous phase when applied to an external field. Cluster analysis has been applied as a method for evaluating the effect of experimental conditions on the structural changes of hybrid borate forms, the grouping of physicochemical quantities and the composite composition of borate glasses, and distinguishing two taxa by morphological parameters. All five articles submitted as habilitation work were published in 2017, and in two of them, Dr. Nedyalkova is a correspondent author.

The monograph included in the competition, *Computational Study of Soft Nanoparticles and Effect of Ions*, was published by the academic publisher Lambert in 2019. Its title is very similar to the title of the candidate's dissertation, *Computer Nanoparticle Research: Effects of Metal Ions, Solvent and Lemon acid*, which also appears in the monograph. The lack of an abstract does not allow me to judge whether and to what extent the same results are presented in the monograph. I noticed a duplication of an article (M. Nedyalkova, H. Hristov, V. Simeonov, "A statistical approach to the study of lithium magnesium metaborate glasses", *Open Chemistry*, 15, 61-66, 2017), included in the habilitation work and then in the list of articles outside of habilitation work. Therefore, the points on indicator D should be reduced from 255 to 235. One of the articles published in the *Journal of AOAC International* 100, 395-364, 2017, according to SCOPUS and Web of Science, is quartile Q3, not Q2, as has noted Dr. Nedyalkova and this leads to a decrease by 5 more points. As a final result on indicator D I define 230 points.

By indicator E, Dr. Nedyalkova presented 30 citations (60 points) on 7 articles. The layout of the evidence is negligent. With few exceptions, the citation publications do not indicate the years of their publication. The names of the authors of all the articles citing the work in *The Journal of Chemical Physics* from 2012, which is not included in the lists of articles in the competition, are missing (only present in the candidate's CV). Some of the citations are not found in the SCOPUS and Web of Science databases, but only in Google Scholar, and this means a decrease in points on this indicator.

From the information provided about the teaching activity of Assist. Prof. Miroslava Nedyalkova makes it clear that she has fulfilled the minimum annual standard of teaching hours of the Faculty of Chemistry and Pharmacy and has one 1 graduate student.

In connection with the mentioned above, I propose that Dr. Nedyalkova to present her scientific contributions in a summarized form and to explain the difference between her dissertation and the presented monograph *Computational study of soft Nanoparticles and effect of ions*.

### **Conclusion**

After getting acquainted with the materials and scientific works presented in the competition, I find that the materials according to the procedure meet the requirements of the Regulations for the development of the academic staff in the Republic of Bulgaria and the regulations of the Faculty of Chemistry and Pharmacy at Sofia University. The Assistant Professor Miroslava Nedyalkova has fulfilled the minimum national requirements in the professional field. After taking up the position of Principal Assistant Professor, she shows a very active publishing activity in reputable journals and after receiving the answers to the questions raised, I would support her application and recommend to the Scientific Jury to submit a report proposal to the Faculty Board of the Faculty of Chemistry and Pharmacy Miroslava Alexandrova Nedyalkova in the academic position of *Associate Professor* in the field of higher education: 4. Natural Sciences, Mathematics and Informatics; professional field: 4.2. Chemical sciences: Theoretical chemistry.

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/Prof. Venelin Enchev/