

REVIEW

by Prof. Dr. Ala Tadjer, member of the Scientific Jury, appointed by the Rector of the University of Sofia for the contest for the academic position “Associate Professor”

announced in the State Gazette no. 52 / 02.07.2019

professional field 4.2. Chemical Sciences (Theoretical Chemistry)

In the contest for the academic position of "Associate Professor" in the professional field 4.2. Chemical Sciences (Theoretical Chemistry), for the needs of the Department of Inorganic Chemistry at the Faculty of Chemistry and Pharmacy of the University Sofia “St. Kliment Ohridski, announced in State Gazette No. 52/02/07, applied just one candidate – Head Assistant Professor Miroslava Alexandrova Nedyalkova, faculty member of the same Department.

Miroslava Nedyalkova was born in 1982. In 2004 she graduated from the Bachelor's program in Chemistry and Physics, and in 2006 graduated from the Master's Program in Pharmacological and Medical Biophysicochemistry, both at the Faculty of Chemistry at Sofia University “St. Kliment Ohridski ". In 2014, she defended her doctoral thesis on "Computational Study of Nanoparticles: Effects of Metal Ions, Solvent and Citric Acid", thus meeting the requirements of **Indicator A** of the minimum national requirements.

From 2007 to 2016, she was an assistant at the Department of Inorganic Chemistry of the Faculty of Chemistry and Pharmacy of Sofia University (FCP-SU). During this period (from 2011 to 2014) she was also a PhD trainee with scientific consultants from the Faculty of Physics of Sofia University and from the University of Barcelona, Spain. Following her defense, a contest for a Head Assistant Professor has been announced at the Department of Inorganic Chemistry of FCP-SU, a position she has been holding since 2017 and currently has over 2 years of experience.

Since 2010, Dr. Nedyalkova has visited annually the University of Barcelona with different lengths of stay and different sources of funding - participation in projects and scholarships of all kinds. Added to this is a one-month specialization in France in 2015 and short-term trainings in Geneva (2015) and Vienna (2017). She is currently in the University of Maryland, Baltimore, USA, with a 6-month Fulbright Foundation scholarship.

In her curriculum vitae, which has not been updated since last year, the candidate lists 22 participations (with strange numbering) in schools, congresses, conferences, workshops, 9 of which are in Bulgaria. In addition to the grants and scholarships won, several awards are listed, the most significant of which is the 2018 L'OREAL-UNESCO “For Women in Science” Award.

With so many specializations and awards listed in the CV and the SU database "The Authors", it is not clear why there is a lack of documentation under item 7 of the application for participation in the contest, namely: "Documents, proving the fulfillment of the requirements under Art. 105, para. 1, item 2 (notes and certificates from an employer, project manager, financing organization or contracting authority, references and reviews, awards and other relevant evidence)."

Dr. Nedyalkova presented a list of all her publications in the scientific periodicals, a total of 29, as well as one chapter in a compendium and one monograph. Among them, she has selected 15 articles and the monograph for the contest, all of them published after receiving her doctoral degree. Of these, 8 are in journals of quartile Q1 and 7 in Q2. She has selected 3 of the Q1 and 2 of the Q2 publications to meet the minimum requirements of the **group B indicators**, and has also presented a habilitation paper. The remaining 10 papers cover and even exceed both the national requirements of **group D indicators** and those recommended by FCP-SU, even without the monograph. A list of 30 citations on the total of 7 articles out of those, with which the candidate participates in the contest, is provided. This is not the complete list of citations, but it is sufficient to meet the minimum national requirements of the **group E indicators**. In fact, the citations on these 15 articles are 46 (without self-citations). 30 of them are on 2 publications - 18 for the review under No. 12 and 12 for the excellent article № 10. The remaining 16 are allocated to other 8 articles, so the quoted articles are a total of 10. It is a good idea for the candidate to update this list in order to cover the recently adopted recommended requirements of the FCP-SU. According to the *Scopus* scientific database, the integral *h*-index of Dr. Nedyalkova (excluding self-citations) is $h = 4$.

Dr. Nedyalkova has significant involvement in 5 projects and in the organization of 4 conferences. All this testifies to her active participation in project financing and in initiatives for establishment of international contacts for joint research. I believe that this should be emphasized markedly.

As an Assistant Professor, she has been conducting Inorganic Chemistry lab classes and working with students on research topics. She has supervised one successfully defended student diploma thesis. Presently, she trains a gifted research student.

These activities, together with the *h*-index, would bring her a significant three-digit score in the newly proposed **G group of indicators** in the recommended requirements for the academic position Associate Professor at the FCP-SU.

All types of documents required by law and the regulations for its implementation are presented, although some of them are not accurately prepared technically. This applies also to some of the submitted manuscripts or publications. For example, the habilitation paper (written in English) requires considerable linguistic and technical editing. Although the text of about 25 pages is mainly based on two published papers (# 9 and # 12 in the contest article list), there are a significant

number of errors and references to non-existent tables, while most of the available tables are named "Figures". More than 100 pages of tables have been added to this really interesting text, without explanation. Of course, the national requirements do not include the compulsory submission of a habilitation paper, but once written, it should have been carefully proofread.

Dr. Nedialkova's scientific career is quite diverse. During her M.Sc. project, related to an experimental study of Langmuir films, she supplemented it with Monte Carlo simulations on her own initiative. She then went on to do quantum-chemical calculations, which she sometimes does to this day, but then reoriented herself to the classic molecular-dynamics simulations that underpin her PhD thesis. However, after receiving the PhD degree, the candidate again changed direction and started applying statistical methods for processing experimental data, namely chemometrics approaches. The papers presented for the contest clearly show her evolution from an "apprentice" to a "master". The publications submitted for the contest are basically of 2 types - in a review form or with purely applied character. The reviews demonstrate the applicant's ability to capture, analyze and synthesize a large amount of scientific information in a very well-organized and fully consistent and comprehensible manner. The applied are dedicated to statistical processing and search for interrelations and / or similarities on the basis of experimental data of different nature and origin. In some cases, these data were collected from the literature, in others (the majority of cases) the data were obtained by collaborators.

Over the past 20 years, chemometrics, with its interdisciplinary nature, has started playing an important role as a research methodology, attracting the interest of a wide variety of scientific and engineering backgrounds. Dr. Nedialkova's publications are a vivid illustration of this statement: systems applied to multivariate statistics methodologies in her papers range from boron glasses to baby products, from air, soil and water pollutants in rivers and seas to botanical identification of plant species, from pharmacy and medical applications to nanoparticle toxicology, from conformational analysis of organic compounds to packaging materials. Of course, in each paper there is a statement that the chemometrics methods sort the information and define dependencies with interpretative and predictive ability without explaining the causation and the mechanism of interaction, but this information is more than useful for the practice.

Almost all publications presented for the contest are with a large team of authors, with participants from different Bulgarian and foreign scientific institutions, which discloses the candidate's ability to work in a team. It is a pity that there are no contribution-distributing conventions and it is impossible to determine Dr. Nedialkova's share - given her diverse qualifications, she could have participated in both the experimental part and the chemometric one. Perhaps, the candidate will shed more light on this question at the closing meeting of the Scientific Jury.

A monograph is presented to meet criterion 5 of Group D (D5. Published monograph containing research not included in the habilitation paper). However, it should rather be referred to criterion 6 (D6. A published book based on a thesis for a doctorate degree), because it is actually Dr. Nedyalkova's PhD thesis from the first to last page. It is useless to comment on its merits and imperfections, because this was done by the members of the Scientific Jury which awarded her the doctoral degree and it is not appropriate to review the reviews and statements of colleagues. In my opinion, this work can be excluded from the contest materials without any risk for failing to meet the criteria for the pursued academic position.

As I have already noted, the contest documents have been prepared with some carelessness. Apparently, spelling and punctuation are not among the candidate's strengths. This is true for both languages, in which the materials are written, and even for the published documents, some of which contain missing words, grammar errors or misused expressions. In contrast, the **Account of the Scientific Contributions** is very well written and meaningful, correctly reflecting contributions to the relevant publication, in particular those contributions related to chemometric estimates, and two things can be judged thereof: first, in what part of the study the candidate was mainly involved, and second, most important of all, that Dr. Nedyalkova has become a true specialist in multivariate statistics and is able to independently choose the most suitable for the system under consideration statistical method and to analyze critically the results. For this purpose, in addition to mastering the chemometrics approaches, the researcher must become familiar with details about the objects of study and with such a wide variety of objects, this is a challenging task that the candidate obviously successfully copes with.

Conclusion

Dr. Miroslava Nedyalkova's indicators cover all the minimum national requirements for the academic position Assistant Professor in the professional field of Chemical Sciences, as described in the Rules for the Implementation of the Law on the Development of the Academic Staff of the Republic of Bulgaria. All additional recommendations of the Faculty of Chemistry and Pharmacy of Sofia University are fulfilled and exceeded. The habilitation paper is well structured and not very well prepared, but is complemented by the corresponding number of publications in scientific journals belonging to quartiles Q1 and Q2. The monograph could also be discarded because the other publications are quite sufficient. It is advisable an evaluation of the candidate's personal contribution in articles by more than three authors to be provided together with an update of the citations and some feedback from the scientific institutions visited, since a considerable part of the

candidate's time and research in the past 9 years has been conducted abroad.. The author's Account of the Scientific Contributions very well and completely adequately reflects the scientific contributions and was written with professionalism.

On the basis of all the above, I support the application of Dr. Miroslava Alexandrova Nedyalkova for the academic position “Assistant Professor: in the professional field 4.2. Chemical Sciences (Theoretical Chemistry).

Sofia, November 8, 2019

Member of the Scientific Jury:

/Prof. Alia Tadjer, PhD/