

# REVIEW

by Prof. Vassil Borissov Delchev, PhD, DSc,

Dept. Physical chemistry, University of Plovdiv

Competition: for the academic position "Associate professor" at the University of Sofia

in area of higher education: 4: Natural sciences, mathematics and informatics;  
Professional field 4.2. Chemical sciences; scientific field "Theoretical chemistry"

Candidate: Chief assist. professor PhD Miroslava Aleksandrova Nedyalkova,  
Dept. Inorganic chemistry, Faculty of chemistry and pharmacy, University of Sofia

---

Announcement of the Competition: *State Gazette* No 52 / 2019

Rector's order for the constitution of the Scientific jury: PД38-446/24.07.2019

Decision of the first meeting of the Scientific jury: to write an academic review

---

The documents applied consist of the next printed matter: 1) a Standard *Curriculum Vitae*; 2) a diploma for higher education (only for the master level study – the appendix is badly scanned and the most of the information is not readable) and a PhD diploma; 3) an annex to the employment contract for the last promotion at the academic position "chief assistant professor" (2 copies); 4) a certificate of work experience; 5) a list of all publications and a list of publications participating in the current competition; 6) a list of publications included in the e-system "The authors"; 7) an information for the implementation of the minimal national requirements; 8) lists of citations and contributions; 9) information according to Art. 112(2); 10) scientific works and abstracts in Bulgarian and English; 11) a monograph as a habilitation thesis; 12) a protocol from the Academic council with a decision for the initiation of the competition for an academic position "associate professor"; 13) a habilitation thesis; 14) a copy of the announcement published in the *State Gazette*.

Among the application forms I did not find the next documents: 1) a certificate of health; 2) a certificate showing no previous conviction. They are applicable according to Art. 107(1) of the Rules for conferment of scientific degrees and appointing of academic positions at the University of Sofia. I hope Dr. Nedyalkova has delivered these documents to the responsible service at the University of Sofia.

## **Biographic information**

In 2004 Dr. Miroslava Nedyalkova has graduated the Faculty of chemistry and pharmacy at the University of Sofia with a bachelor's degree, subject "Chemistry and physics". No diploma for this educational level has been enclosed in the documentation! In 2006 she has graduated with a master's degree; subject "Chemistry", professional qualification "Master in medicinal and pharmacological biophysical chemistry". In 2013 Dr. Nedyalkova has defended successfully her PhD thesis and she has been awarded a doctoral degree in theoretical chemistry. The title of the PhD thesis is "*Computational study of nanoparticles: effect of metal ions, solvent and citric acid*". Because of the quite general title I expected to find, among the documents, the abstract of the PhD thesis!

In the period 2007 – 2006 the applicant has held the position "assistant professor". For 2017 until now she has been promoted to a position "chief assistant professor" at the department of Inorganic chemistry of the Faculty of chemistry and pharmacy (University of Sofia). Dr. Nedyalkova has visited research groups in Spain, France and Switzerland. The terms of the visits vary from several days to several months. Dr. Nedyalkova has participated in activities at the Vienna University of Technology, in the research group of prof. Schwarz. The aim of the visit has been to introduce her to the program – Wien2k – software for investigation of the electron structure of solids by means of DFT methods. A good impression

makes the great number of awards that the applicant has been awarded from different institutions. She is a member of nine organization committees of conferences and projects.

### **Scientific activity**

#### *Scientific works*

Dr. Nedyalkova presented 16 printed scientific works in the competition for the position “associate professor” – one book and fifteen scientific papers. One habilitation thesis entitled „*Multi-scale modeling approach towards the development of nanoQSAR by hemometrics methods*” is also applied. It has been presented in the Faculty of chemistry and pharmacy at the University of Sofia. The scientific investigations of the applicant are based on three major approaches – chemometric, molecular dynamical and quantum chemical. With regard to the methods applied and the objects of investigation, the scientific contributions have rather particular character. In other words in the scientific papers are reported results based on a diversity of methods and objects, which makes difficult to deduce some general contributions. Listed by papers, the next particular contributions can be mentioned:

1) The partition coefficients of a group of polar solvents in the heterogeneous systems water/octanol and air/octanol have been determined at the DFT theoretical level including a solvent model (paper 1). At the same level, the geometry structures and the NMR properties of  $\alpha$ - $\text{MnC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$  and  $\gamma$ - $\text{MnC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$  have been studied, while the dehydration process of  $\text{MnC}_2\text{O}_4 \cdot 3\text{H}_2\text{O}$  has been investigated with molecular dynamics (paper 4). The conformers of citric acid have been also explored by means of quantum chemical calculations. It has been found a low energy barrier explaining the process of intramolecular H-transfer in the compound (paper 11). The (in)stability of a thin toluene emulsion film in contact with the water phase has been estimated by means of molecular dynamics simulations. The mechanism of the film rupture has been proposed at NVT and NPT (paper 10).

2) Cluster analysis has been applied for 1400 food proteins and further they were classified as allergenic and non-allergenic (paper 2). An assessment of pollution in the region of a metallurgical combine near Plovdiv has been done using multivariate statistical methods (paper 3). Regression models have been found which render an account of the relationship between the ecotoxicity of packaging material and different experimental conditions of conservation and processing of packings (paper 5). Some physicochemical properties of “green” solvents have been found by clustering chemometric tools (paper 6). The relationship between the experimental conditions for extraction procedures of some baby products and the ecological response when tested by various ecotoxicity tests has been established (paper 7). The influence of the experimental conditions on the structural changes of some nanocomposites has also been clarified by cluster analysis (paper 8). A classification of systems of nanoparticles has been done. The relationship ecotoxicity – physicochemical properties has been assessed (paper 9). With multivariate statistics an attempt has been done to distinguish two taxa by morphological features (paper 13). Some physicochemical properties and the composite composition of borate glasses were classified by cluster analysis (paper 14). The ecotoxicity of drugs has been evaluated by correlation analysis (paper 15).

Paper 12 is a review. A detailed review of some medical applications of iron oxide nanoparticles has been done with the point of view of their toxicity and their applicability in medical diagnostic. The paper is based on 281 references. I would like to know the personal contribution of the applicant in this work.

Most of the papers have a large number of co-authors and in the list of contributions enclosed to the application forms it is not clear what is the personal contribution of Dr. Nedyalkova in all those investigations. Since I don't have any preliminary contacts with Dr. Nedyalkova and her science, I find it difficult to answer what part of the investigations in each paper is her personal achievement. I importunately ask the applicant to supply this information.

The review of the papers led to some questions. They are connected in most cases with the choice of a theoretical level for the computations performed and the solvent model. In many cases a motivation for the application of a given quantum chemical method (DFT or MP2) and a base set is absent or poorly explained (for the study of H- bonds the use of diffuse functions of the heavy atoms and hydrogen atoms is highly recommended). I recommend the candidate in her future studies to motivate in details the accuracy of the computational level and the base set used.

Another question is related to the results reported in paper 4. The authors have reported that they have found a crystal structure of crystalhydrates of manganese oxalate according to calculations performed at the DFT level. However I didn't find any parameters of the unit cells in the print. Only the spatial symmetry group of  $\gamma$ - $\text{MnC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$  has been given –  $P2_12_12_1$  (a primitive orthorhombic Bravais unit cell). Furthermore on Fig. 2 in paper 4 it is hard to distinguish three screw axes  $2_1$ .

According to the minimal national requirements in the professional field of the competition, for indicator B, Dr. Nedyalkova has presented five publications equivalent to one habilitation thesis. Three of them have quartiles Q1 and two of them - quartiles Q2. The total score for this parameter is 115 points. It exceeds the minimum of 100 points required in the minimal national requirements.

Dr. Nedyalkova has given ten publications for indicator  $\Gamma$ . Five of them are in scientific journals with quartiles Q1 and they are published in impact scientific journals with high IF - over 3. I would like to point out that the impact factors of the journals in which the candidate has publications are not given in the application documents. Although it is not required in the minimal national requirements, the IFs of the journals with publications one scientist are a touchstone for the position of one scientist in the world scientific community.

The papers with quartiles Q1 have  $\text{IF} = 22.17$ , that is a really impressive achievement for one young scientist.

Four of the papers for indicator  $\Gamma$  are published in journals with quartiles Q2. One paper is published in a journal with a quartile Q3 (according to Scopus and WoS) and not with a quartile Q2 as it is declared by the candidate. This is the article published in *Journal of AOAC International*, 2017, 100:2, 395–364. In that case I reduce the number of points for indicator  $\Gamma$  from 255 to 250 pts.

Dr. Nedyalkova participates in the competition for the academic position “associate professor” with one monograph – a book entitled „*Computational study of soft Nanoparticles and effect of ions*”, published in Lambert academic press (ISBN 978-3-659-87210-5, 2018). Because of the absence of the dissertation abstract, it is hard for me to judge to what extent this monograph repeats the works used for the PhD thesis. I'm expecting the applicant to provide information about that.

#### *Participations in scientific events and projects*

Dr. Nedyalkova has participated in scientific forums in Bulgaria and abroad. She has presented 34 oral reports. She has participated in a large number of projects – 18 being a project team leader on five of them. The applicant is a member of the teams of three activities of the ERASMUS+ program.

#### *Citations*

As for indicator  $\Delta$ , the applicant participates in the competition for the academic position “associate professor” with 30 citations. From the documents applied it is not clear whether some of the citations have been used in the procedures for the PhD degree and for the academic position “chief assistant professor”. For example, some of the citations that are applied in the present competition are from the year of the PhD thesis defence and it is hard to decide whether these citations have been used in the procedure (according to the Rules for

the application of the Law for development of the academic staff - rider 76 and 9). I would like the applicant to clarify this problem. In the citation list there are some citations on a paper that is not included in this competition (*J. Chem. Physics*, 2012, 137:17, 174701).

The search in the online bases SCOPUS and WoS of all publications of the applicant for the period 2012-2019 showed a Hirsch index = 4. I hope that this index will be increased in future since now it has a quite limited value for the position which the applicant applies for. The most cited article is *Advances in Colloid and Interface Science*, 2017, 249, 192-212 (in SCOPUS) with 18 citations - only 13 of them are included in the present procedure.

I reduce the points for indicator  $\Delta$  with 4 (from 60 pts to 56 pts). The reasons are the following: citation 7 of paper [2] and citation 2 of paper [2] cannot be found in SCOPUS and WoS and should be valued with one point only; citation 1 of article [6] is unclear and incomplete and for that reason I reduce the citation list with it.

### **Teaching activity**

The information provided for the teaching activity of Dr. Nedyalkova is quite limited. For the period 2016-2019 Dr. Nedyalkova covers the minimal year quota for the teaching staff of the Faculty of chemistry and pharmacy at the University of Sofia. The teaching activity of the applicant as a chief assistant professor comprises lecture courses and laboratory exercises. Dr. Nedyalkova has been a lecturer of undergraduates-bachelors for the lecture courses of "Solid state chemistry 2" and "General and inorganic chemistry 2". She has supervised a laboratory practicum in "General chemistry and stoichiometry" and "General and inorganic chemistry 2" (for non-Bulgarian undergraduates) at a bachelor's level. Dr. Nedyalkova is a diploma work supervisor of one diploma student and a consultant of one dissertation thesis.

I expected the number of diploma students of the applicant to be larger for the teaching period. There is no information in the documents applied for the participation of the applicant in master's level programs. If there are such activities I would expect to be provided. There is no information for the participation of Dr. Nedyalkova in the preparation of handbooks and lecture courses for disciplines in the Faculty of chemistry and pharmacy.

I recommend the candidate to be more active in the teaching in the department of Inorganic chemistry in the Faculty of chemistry and pharmacy at the University of Sofia and also to strain efforts for the preparation of new lecture courses including the theoretical methods used in her scientific research.

### **CONCLUSION**

The materials provided are in agreement with the Law for development of the academic staff in Republic of Bulgaria and the Rules for its application. The candidate covers the minimal national requirements in the professional field. She has achievements in her scientific field and after providing the missing information mentioned above, I would be prone to give a positive vote for her candidature and to recommend to the Scientific jury to propose to the Faculty council of the Faculty of chemistry and pharmacy at the University of Sofia to elect chief assistant professor Dr. Miroslava Nedyalkova to the academic position "associate professor" in area of higher education: 4: Natural sciences, mathematics and informatics; professional field 4.2. Chemical sciences; scientific field "Theoretical chemistry".

25.10.2019  
Plovdiv

Reviewer: