STATEMENT

by Professor Konstantin Todorov Balashev, DSc

for the contest of the academic position "Professor" in professional field 4.2. Chemical sciences for the scientific specialty "Theoretical Chemistry - Computational Chemistry", for the needs of the Faculty of Chemistry and Pharmacy of SU "St. Cl. Ohridski", announced in State Gazette No. 21 of 15.03.2022, with a candidate

Assoc. Prof. Dr. Galya Kostova Madjarova

1. General requirements and brief description of the candidate

Associate Professor Galya Kostova Madjarova participated as only one candidate in the Professor of Theoretical Chemistry - Computational Chemistry contest at the Faculty of Chemistry and Pharmacy, Sofia University. Associate Professor Madjarova graduated in 1995 from the Faculty of Chemistry, Sofia University “St. Kl. Ohridski" with a Master's degree in Chemistry, specializing in Chemical Physics and Theoretical Chemistry. After that from 1996-1999, she was a Ph.D. student and successfully defended his doctorate in Theoretical Chemistry, in 1999. Her academic career began in 2001, when she was selected as an assistant professor at the Department of Physical chemistry, Faculty of Chemistry, Sofia University. Then, after acquiring the academic positions of Senior assistant (2002-2005) and Chief assistant professor (2005-2013), 2013 she was tenured as an Associate professor in the same department, a position she currently holds. She held numerous temporary positions as a postdoc or researcher at leading universities and research institutions in Germany, Japan, France, and Great Britain.

2. Description of the presented materials

Associate Professor Madjarova has prepared and presented in tabular form a report on the fulfillment of the minimum national requirements for the scientific position "professor". She participates in the contest with a scientific production of 41 publications, mostly published in leading specialized international journals. As of today (07.07.2022) in the database "Scopus" can be found 31 of her articles with 436 citations. Her Hirsch index is 13, excluding self-citations by all co-authors.

The presented list of 11 publications (appendix 3) for participation in the contest includes publications that fully match the subject of the announced contest. They are predominantly published in renowned and leading journals in the field of theoretical chemistry, such as The Journal of Physical Chemistry B, Journal of Chemical Theory and Computation, Applied Physics, Journal of Molecular Liquids, etc.

Associate Professor Madjarova presented a 92-page habilitation thesis on the topic titled: "Design of new hard magnetic materials without the use of rare earth elements", where she summarized her main scientific contributions to the theoretical modeling of materials, which have a strong applied significance. She has been an active participant in

many scientific projects funded by Sofia University, the Ministry of Education, or European and international programs, and in 6 of them, she was the leader after her habilitation.

The indicators for the academic activity of Associate Professor Madjarova significantly exceed the minimum national requirements and those of the Faculty of Chemistry and Pharmacy for the scientific activity of the candidates required for the academic position “Professor.” This is shown in the table:

Group indicators	National requirements	Requirements of the Faculty of Chemistry and Pharmacy	Point acquired by the candidate
А	50	50	50
В	100	100	100
Г	200	220	257
Д	50	60	258
Е	150	150	270
Ж	-	120	160

3. General characteristics of the research, pedagogical and applied research activities of the candidate

Associate Professor Madjarova's research is in two scientific areas of theoretical chemistry - atomistic molecular dynamics simulations and quantum chemical methods for modeling and application of machine learning methods. Her educational and teaching activities are as a lecturer in key courses, such as Structure of Matter, Molecular Modeling of Materials, Quantum Chemistry and Molecular Mechanics, Theoretical Chemistry and Applied Computational Chemistry, which are part of the undergraduate programs of the majors, Chemistry, Ecological chemistry, etc. in the Faculty of chemistry and pharmacy of Sofia University. Prof. Madjarova has supervised four graduate students who successfully defended their master's or bachelor's theses, and she is currently the supervisor of a doctoral student enrolled in 2021.

4. Main scientific and applied scientific contributions

The contributions of Associate Professor Madjarova can be systematized according to the above-mentioned areas of her research, as follows:

• Investigation of the supramolecular structural organization of the inverted hexagonal mesophase composed of glycerol monooleate (GMO), tricaprine and water, (*Articles [1,4] of Appendix 10B*).

• Study of the spontaneous aggregation of a series of salts of bile acids in aqueous solution, the factors for the formation of primary micelles from their salts and the structure of the aggregates obtained in the course of molecular dynamics simulations (*article [2] of appendix 10B*).

• A mechanism for coupling active drug delivery systems that are based on folate or antifolates, with modeling of all components of the active drug transport system, to the α-folate receptor (FRα), (*articles [7 -11] from Annex 10B*).

• The application of time-dependent density functional theory (TDDFT) to the calculation of the excitation spectrum of molecular crystals and 1D polymers in the molecular crystals of picene, pentacene and the 1D-polymer poly(p-phenylenevenylene), (*articles [2] of appendix 10B*).

• Modeling of the magnetic properties of permanent magnets without rare earth elements in the structure. The magnetic properties of Heusler alloys were studied and the possibility of tetragonal [5] and hexagonal deformation was evaluated (*articles [6] of appendix 10B*, monograph).

7. Personal impressions of the reviewer about the candidate

I have known Associate Professor Madjarova since the years when both of us were doctoral students in the Department of Physical Chemistry. I have always highly valued her competence as a specialist and responsiveness as a colleague. Especially useful for me were the many and fruitful discussions we had at the seminars of the department or these that we have during our joint participation in some of the scientific projects of the Faculty of chemistry and pharmacy.

CONCLUSION

The documents presented by Associate Professor Madjarova, as the only candidate for the announced contest for the academic position "Professor", satisfy and exceed the requirements of the Law and the recommended criteria of the of Faculty of Chemistry and Pharmacy, Sofia University. Her contributions are undeniable and evidently distinguishable in the scientific community.

The analysis of her overall research work, and scientific and pedagogic activities give me reason to support Galya Kostova Madjarova's candidacy and to recommend to the members of the respected scientific Jury and to the Faculty Council of Faculty of Chemistry and Pharmacy to award her the academic position "Professor" in a professional field 4.2. Chemical sciences for the scientific specialty "Theoretical Chemistry - Computational Chemistry".

11th July 10, 2022, Sofia

(prof. Konstantin Balashev, DSc)