REVIEW

from Prof. DSc Sonia Varbanova Ilieva,
Faculty of Chemistry and Pharmacy, Sofia University “St. Kl. Ohridski"
of the materials submitted for the competition for the academic position of **'Professor'**
in the Faculty of Chemistry and Pharmacy, Sofia University “St. Kl. Ohridski",
higher education professional field 4.2. Chemical Sciences (Theoretical Chemistry – Computational Chemistry)

In the competition for the academic position **'Professor'** announced in the State Gazette, issue 21/15.03.2022, **Associate Professor Dr Galia Kostova Madjarova** from the Faculty of Chemistry and Pharmacy, Sofia University is the only candidate.

General presentation of the materials deposited

The materials submitted by Assoc. Prof. Galia Madjarova **meet all the requirements** of the Law for the Development of the Academic Staff in the Republic of Bulgaria and the relevant regulations for its implementation (including those of Sofia University and Faculty of Chemistry and Pharmacy). The applicant meets and exceeds the criteria (minimum requirements) of the Faculty of Chemistry and Pharmacy for the academic position "Professor".

Assoc. Prof. Madjarova has published a total of 42 scientific papers (more than 330 citations, h index 12) and for the participation in this competition she has submitted 11 publications in scientific journals (86 citations) and a monography that do not repeat the ones presented in other competitions for occupying academic positions and obtaining scientific degrees. Submitted publications are distributed among the relevant Q factors as follows: 9 - Q1; 1 - Q2; 1 - Q4.

The candidate has submitted a monograph “Design of new hard magnetic materials without the use of rare earth elements”. The presentation of the scientific results in the monograph is accompanied by a brief discussion of the place of the relevant developments in a given scientific field as a whole and their contribution in solving specific problems in the field.

A report for the scientific contributions of the research work is presented. The main scientific contributions of Assoc. Prof. Madjarova are discussed in the report in a concise and clear manner.

Brief biographical information

G. Madjarova graduated as a Master of Sciences in Chemical Physics and Theoretical Chemistry at the Faculty of Chemistry, Sofia University “St. Kl. Ohridski” in 1995. In 1999 she defended her doctoral thesis on the topic "Structure of one-dimensional polymers with magnetic properties". Then she continued her scientific work at the Faculty, Department of Physical Chemistry as an Assistant (until 2005) and subsequently Chief Assistant (2005-2013). Since 2013 she has held the academic position of Assistant Professor in the same laboratory. Therefore, the professional and scientific experience gained is fully linked to the announced competition.

Assoc. Prof. Madjarova has specialized in foreign research groups - Max Planck Institute of Microstructure Physics, Halle, Germany, University of Hull, UK, Institute for Chemistry of Surfaces and Interfaces, Mulhouse, France, Institute for Fundamental Chemistry, Kyoto, Japan; University of Leipzig, Germany. After these visits, the collaboration with colleagues from abroad continued that is evident from the published co-authored scientific papers.

She has participated in a number of national/international scientific congresses/conferences and research/educational projects. She participated in 12 national and 2 international projects; she is the head of 6 projects financed specifically from the state budget (Sofia University Science Fund). She is the co-supervisor of the Laboratory for Modeling and Prediction of Processes and Properties of Materials for Clean Technologies at the National Center for Mechatronics and Clean Technologies.

Her teaching activity is rich and diverse and is expressed in the management of graduates: supervision of 4 bachelor graduation theses and co-supervision of 6 master degree theses; scientific consultant of 1 doctoral thesis; co-supervisor of 1 PhD student enrolled 2021, as well as regular teaching activities in the Faculty. Currently Assoc. Prof. Madjarova is the Vice dean at the Faculty of Chemistry and Pharmacy.

General characterization of the applicant's scientific activities

The applicant's overall scientific activity is in the field of theoretical chemistry that is completely in line with the announced competition. Scientific publications submitted for participating in the competition reflect the work of Dr Madjarova in the following scientific area: **modeling of structure and properties by theoretical methods – molecular dynamics simulations and quantum chemical calculations.**

Molecular dynamics simulations have been applied to study various structures related to biological processes in the body, their supramolecular organization, processes of aggregation, micelle formation, hydrophobic interactions, formation of hydrogen bonds, tautomeric properties, etc. The considered biological processes are primarily related to the transport of molecules through the double lipid layer of the cell membrane. That is why lipid systems are the subject of research in the work of G. Madjarova and the team she is working with. Two of the published scientific articles (1 and 4) are devoted to one of the most interesting and promising new lipid systems – an inverted hexagonal mesophase made of glycerol monooleate (monoolein) and water. Monoolein-based HII mesophases have been the subject of research in the scientific literature regarding their structural properties and their potential application in the "control and management" of bioactive macromolecules such as lysozyme and insulin. In the work of Dr Madjarova and the team, the structure of the elementary cell has been established. The influence of added tricaprylin on the stability of the structure has been studied and its stabilizing effect on the system - explained. The ability of these systems for self-organization is of particular interest. As a result of the self-organization process the system can accept larger sized molecules (larger than the diameter of the channel). That is why this type of systems have the potential for application in the field of drug delivery systems. Experimental studies have been conducted by Prof. Garti, Hebrew University of Jerusalem, Israel.

A number of studied folate-based drug delivery systems have been published in the scientific literature, but the mechanism of binding of the ligand or its derivatives to the receptor is not fully

understood at molecular level. Research on the molecular structure and dynamics of folate and antifolates has been carried out by Dr Madjarova. The tautomeric equilibrium in solution for the folate isomers has been studied, the folate receptor has been characterized through the combined application of experimental and theoretical methods. A model of a cell membrane has been proposed - a bilayer consisting of different lipids. The model has been applied for clarifying the binding mechanism of three ligands to the active center at the molecular level.

Elucidation of the mechanism of interaction has been applied to explain experimentally observed differences in the affinity of the series of ligands to the receptor. Dr Madjarova emphasizes in her contributions report that such a detailed atomistic model of the cell membrane has been presented for the first time in the literature. The work on this topic has been carried out by a team. Galia Madjarova has participated in the entire research process.

Quantum chemical calculations have been applied to theoretically solve physical problems in studying the change and sensitivity of molecular crystals to alternating electric fields. TDDFT formalism has been applied to calculate the excitation spectra of various materials. Magnetic properties of permanent magnets have been modeled. A new approach has been published for constructing new solid magnets by forming stacks of existing binary magnets in order to increase the magneto-crystalline anisotropy while attempting to reduce the amount of expensive metal and replace it with a cheaper one. Based on this combined approach, several new materials with potentially good properties as hard magnets have been proposed.

The subject of **the monograph** presented is on searching and predicting new materials - hard magnets, which do not contain rare earth elements. The topic is particularly relevant in light of the importance of hard magnets in industry on the one hand, and on the other - the economic and political problems that the process of producing rare earth elements poses. The model systems studied are from the family of Heusler alloys – alloys possessing ferromagnetic properties without containing magnetic elements.

Quantum chemical modeling of two series of Heusler alloys has been carried out. The electronic structure and main characteristics of the studied hard magnets have been calculated by applying Density Functional Theory (DFT). The application of quantum chemical calculations to characterize magnetism is not a trivial procedure. In the process of the study some challenges have been solved, spin-polarized calculations have been carried out, non-collinear approaches have been used, in addition to the ferromagnetic arrangement, antiferromagnetic states have also been studied, and a protocol has been created for calculation and detailed analysis of the properties of materials - hard magnets. From the studied systems, a structure has been determined for which the calculated characteristics are optimal and, in this sense, it can be considered as a potential candidate for the realization of a hard magnetic material.

The second part of the monograph is dedicated to the study of the relationship between the composition of the structures and their magnetic properties with the aim to obtain a quantitative dependence to be used for calculating (predicting) characteristics of magnetic systems in a theoretical way. Availability of databases for modeling of hard magnets is quite limited. An overview of the available databases is made, a comparative analysis - done, and the Materials Project database - used. A decision

tree method has been applied for classifying data. As far as the derivation of the model does not actually use data from the quantum chemical calculations performed, I would like to ask whether an option for a quantitative structure-activity model based on the results from quantum chemical calculations has been considered?

It is evident from the presented publications that Assoc. Prof. Madjarova has continued the research on modeling properties of magnetic systems by expanding and enriching them, and on the other hand, she has developed new topics: application of molecular dynamics simulations for research of structural organization and binding dynamics of drug complexes with receptors; application of machine learning methods for characterizing structure-composition-properties relationships. In her work, she has established fruitful collaboration with colleagues from FCP-SU; the group of prof. Gross, Max Planck Institute of Microstructure Physics, Halle, Germany, Prof. Garti and colleagues at Hebrew University, etc.

I would like to emphasize the interdisciplinary nature of the scientific work of Dr Madjarova that is confirmed by the above discussion and the published scientific papers. The research focus has been on the theoretical calculations, but in accordance with experiments, parallel studies, and potential for application in various scientific fields. I would like to note the rather expanded palette of theoretical methods and software products used in the scientific research on various objects. In my opinion, that is the strongest proof for the continuous scientific growth of G. Madjarova, and therefore the professor position is a natural result in her scientific career.

G. Madjarova is the leading/co-corresponding author in 2 out of 11 scientific works submitted for the competition. 86 citations of the publications in the scientific literature ape noted. The average impact factor of the publications is 3.4, ranging from 1.472 (*European Biophysical Journal with Biophysics Letters*) to 6.006 (*Journal of Chemical Theory and Computation*). I consider that when presenting a list of publications, the main author(s) (corresponding author) should be noted (for instance with a star symbol) as accepted and established in the scientific literature. In fact, this is also determined by the additional requirement No. 2 of the FCP (The candidate has to be a leading scientist in a certain scientific field, demonstrated by at least 5 publications in which he is the first or corresponding author).

The research carried out and the published results have scientific as well as applied contributions in the relevant fields of science. These contributions can be formulated as: substantiations of significant new sides of already existing scientific fields, problems, theories, hypotheses by means of new methods and approaches; creating new methodologies for analysis; getting new facts. These contributions are corroborated by reputable international scientific journals in which the articles have been published, as well as by citations in the scientific literature. The total number of citations is 330, 86 of which are on the publications submitted for this competition. Therefore, the research work of Assoc. Prof. Madjarova is in topical areas of scientific knowledge, with issues that are widely recognized in the scientific community, and the results achieved have high impact scientific contributions.

The scientific results have been disseminated through participations of Dr Madjarova and her colleagues from the group in national and international scientific forums with posters and oral presentations. For the period 2013-2020 Prof. Madjarova has had oral presentations given at 17 scientific conferences, 4 of these being reported by herself.

The educational and pedagogical activity of the candidate is extremely replete and diverse. She has been the lecturer in the following courses: Structure of matter for students in two Bachelor majors, Molecular Modeling of Materials, Theoretical Chemistry, Quantum Chemistry and Molecular Mechanics, Applied Computational Chemistry. Her average annual classroom employment is over 350 hours, and for the academic 2021/22 year this number is 525. She has been the supervisor of 4 diploma theses and currently is the co-supervisor of 1 PhD student. I would like to emphasize the competence, responsiveness and collegial approach in the work of Associate Professor Madjarova.

CONCLUSION

According to the submitted materials and scientific papers, the above analysis of their importance and scientific contributions, as well as my personal opinion about the candidate as a highly erudite scientist, I am convinced in my **positive assessment** and firmly recommend to the Scientific Jury to prepare a report-proposal to the Faculty Council for the selection of Assoc. Prof. **Dr Galia Kostova Madjarova**, for the academic position of **'Professor'** in the professional field 4.2. Chemical Sciences (Theoretical Chemistry – Computational Chemistry) at the Faculty of Chemistry and Pharmacy, Sofia University “St. Kl. Ohridski".

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