O P I N I O N

on the competition for the academic position of **Professor** at the Faculty of Chemistry and Pharmacy of Sofia University "St. Kliment Ohridski" in the professional field 4.2. Chemical Sciences (Theoretical Chemistry-Computational Chemistry), announced in SG, issue 21 / 15.03.2022, with candidate

Associate Professor Dr. **Galia Kostova Madjarova**

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In the competition for Professor in professional field 4.2. Chemical Sciences (Theoretical Chemistry-Computational Chemistry) at the Faculty of Chemistry and Pharmacy of Sofia University "St. Kl. Ohridski" one candidate participates - Associate Professor Dr. Galia Kostova Madjarova. To participate in the competition, the candidate has submitted a complete set of documents in accordance with the requirements of the Regulations for the implementation of the Academic Staff Development Act in the Republic of Bulgaria and the Regulations for the acquisition of scientific degrees and academic positions at Sofia University "St. Kl. Ohridski".

Biographical reference

Associate Professor Galia Madjarova is a graduate of the Faculty of Chemistry of the University of St. Kl. Ohridski", where in 1995 she received the Master's degree in Chemistry (Specialization: Chemical Physics and Theoretical Chemistry). In 1997 she acquired the qualification of Teacher of Chemistry and Chemical Technology. In 1999, under the guidance of Prof. Nikolay Tyutyulkov and Prof. Alya Tajer, she successfully defended her doctoral dissertation on the topic "Structure of 1D polymers with magnetic properties". She began her professional career in 2001 as an assistant professor of theoretical chemistry at the Department of Physical Chemistry of the Faculty of Science of SU, where she successively rose to senior assistant (2002), chief assistant (2005) and associate professor (2013). She specialized in renowned research centers such as the Max Planck Institute of Microstructure Physics, Halle, Germany; University of Hull, Great Britain; Institute for Chemistry of Surfaces and Interfaces,

Mulhouse, France; Institute for Fundamental Chemistry, Kyoto, Japan and University of Leipzig, Germany.

Scientometric data

For the competition, Associate Professor Madjarova has presented 11 scientific publications and 1 monograph, which were published after the defense of her doctoral dissertation and the held competition for associate professor. All publications are published in reputable refereed international journals (e.g. J. Chem. Theory and Computation, J. Phys. Chem. B, J. Mol. Liquids, Phys. Chem. Chem. Phys.) with impact factor and quartile (of them 9 with Q1, 1 with Q2 and 1 with Q4). 86 independent citations were noted on these works. Six of the presented articles were produced in collaboration with foreign scientists. In general, Assoc. Prof. Madjarova is a co-author of 41 publications, the results of which have been cited more than 330 times in the scientific literature. The candidate's Hirsch index is 12. The results of Assoc. Prof. Madjarova's research have been presented in 69 sectional reports at national and international scientific forums. The candidate actively participates in national/international scientific projects (32 in number), being/was the head of 9 of them. From the provided reference, it can be seen that Assoc. Prof. Madjarova meets (and in a number of cases significantly exceeds) the minimum national requirements for the academic position of Professor under Art. 2b from ZRASRB for scientific field Natural sciences, mathematics and informatics, professional direction 4.2. Chemical Sciences, as well as the Faculty of Chemistry and Pharmacy recommended criteria. There is no evidence of plagiarism in the candidate's publication activity.

Scientific contributions

Assoc. Prof. Madjarova's research is focused on the theoretical modeling of the structure, electronic properties and thermodynamic characteristics of chemical/biochemical objects of interest to electronics, pharmacy and medicine. They can be summarized in the following directions:

1. *Atomistic molecular dynamics simulations of biologically relevant structures.* Through the application of state-of-the-art molecular dynamics simulations, new light has been shed on the structural features of the system glycerol monooleate, tricaprin and water (with and without the addition of tricaprylin). The ability of the studied system to transfer biomolecules was evaluated. The mechanism of spontaneous aggregation of another lipid system - bile salts - in aqueous solution

was also investigated, and the physical regularities governing the process were determined. In a series of works, a folate/antifolate-based multicomponent biological system for active drug transport to the alpha-folate receptor was explicitly modeled and investigated. For the first time in the literature, a detailed constitutive atomistic model of a cell membrane was constructed and validated, allowing to observe the spontaneous binding of folate, raltitrexed and 5-methyltetrahydrofolate to the active site of the receptor. The factors determining the experimentally established differences in the affinity to the receptor of the series of ligands were clarified.

2. *Quantum chemical methods for modeling and application of machine learning methods.* By applying time-dependent density functional theory (TDDFT), the excitation spectrum of molecular crystals of picene and pentacene and the 1D-polymer poly(p-phenylenevenylene) was modeled. The analysis of the obtained results shows that the used formalism represents a reliable alternative for a quick evaluation of the excitation spectra of different materials. Of particular interest is the modeling of the magnetic properties of permanent magnets without rare earth elements. The possibilities of Heusler alloys for creating highly efficient magnets have been convincingly demonstrated. In the monograph "Design of new hard magnetic materials without the use of rare earth elements" the factors influencing the magnetic properties of hard magnets were systematically studied. Machine learning methods were applied to search for the "composition-structure-properties" relationship in these materials. Based on a Decision Trees algorithm, a model composed of 14 parameters was proposed, which is capable of qualitatively and semi-quantitatively predicting the total magnetic moment of the unit cell of an arbitrary structure using information about the fundamental properties of the elements, making up the composite. The obtained results can be used as guiding principles in the design/synthesis of high performance solid magnets without the participation of rare earth elements.

Teaching activity

Assoc. Prof. Madjarova is an established and respected teacher at the Faculty of Chemistry and Pharmacy with a high reputation among students and colleagues. She has developed / leads lecture courses on Structure of Matter (Bachelors), Theoretical Chemistry (Bachelors), Molecular Design (Bachelors), Molecular Modeling of

Functional Materials (Bachelors), Quantum Chemistry and Molecular Mechanics (Bachelors), Applied Computational Chemistry (Bachelors) , and Quantum Chemistry and Spectroscopy (Bachelors). She was the supervisor of 4 successfully defended diploma students and co-supervisor of one PhD student.

Conclusion

The publications and monograph presented by the candidate are on the topic of the competition and represent original scientific developments with a significant contribution in the field of theoretical computational chemistry and molecular modeling. The materials provided give me reason to believe that Assoc. Prof. Madjarova is a leading scientist in her field with deep knowledge and practical skills in using state-of-the-art theoretical approaches for research at a high scientific level of complex chemical/biological systems with application in electronics, pharmacy and medicine. The results obtained by the candidate are innovative in nature and represent novelties in scientific research. In her research activity, the candidate demonstrates precision, creative thinking and the ability to select and successfully solve tasks with a high impact for fundamental and applied science.

As a result of the above, I am convinced that with her varied research and teaching activities, Assoc. Prof. Dr. Galia Kostova Madjarova fully meets all the requirements of the Law on holding the academic position "Professor". I propose that Assoc. Prof. Dr. Galia Kostova Madjarova be elected as a Professor in professional direction 4.2 Chemical Sciences (Theoretical Chemistry-Computational Chemistry) at the Faculty of Chemistry and Pharmacy of SU "St. Kliment Ohridski".

18.07.2022

Sofia

(Prof. Todor Dudev)