

Review

on the presented materials of Assoc. Prof. Dr. Galia Kostova Madjarova for participation in the competition for professor in Professional field 4.2 Chemical Sciences (Theoretical Chemistry - Computational Chemistry), at the Department of Physical Chemistry, Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski", announced in the State Gazette, no. 21 of 15.03.2022, by Prof. DSci. Boris Simeonov Galabov

Galia Kostova Madjarova obtained her higher education in the five-year course majoring in Chemistry in 1995 at the Faculty of Chemistry of Sofia University. In 1999, she successfully defended her dissertation in the field of computational and theoretical chemistry under the supervision of Prof. Alya Tadjer. Since 2001, she has been an assistant at the Department of Physical Chemistry of the FHF, later a senior assistant and chief assistant. In 2013, she was elected as Associate professor. Assoc. Prof. Dr. Galia Madjarova has so far published 40 scientific articles and a monograph, mostly in established international scientific journals. Her works have been cited more than 330 times in the specialized literature. Assoc. Prof. G. Madjarova participates in the competition for professorship with 11 publications and the monograph "Design of new hard magnetic materials without the use of rare earth elements" recently published by the Publishing House of Sofia University. Of the presented scientific works, 9 are in a journal from quartile Q1, and the remaining two - in Q2 and Q4. These scientific works, published in the period 2014-2022, were cited a total of 86 times. The candidate has presented a total of 69 reports at international and national scientific conferences as oral presentations and posters. She has participated in 12 national and two international scientific projects. She was the supervisor of 6 scientific projects funded by Sofia University. G. Madjarova was a postdoctoral fellow at the Institute of Fundamental Chemistry, Kyoto, Japan, and a long-term fellow at the Max-Planck Institute for Microstructural Physics, Halle. She has also been on short-term scientific visits to several Western European laboratories. The above-mentioned data outline the candidate in the competition, Assoc. Prof. Dr. Galya Madzharova, as an established scientist with scientific works in leading journals in the field of chemistry and a solid reputation in the international scientific community.

Assoc. Prof. Dr. Galia Madjarova is one of the highly committed teachers in the field of computational and theoretical chemistry. Over the years of her academic career, she participated as a lecturer and seminar supervisor in the following courses: Structure of Matter,

Theoretical Chemistry, Molecular Design, Molecular Modeling of Functional Materials, Quantum Chemistry and Molecular Mechanics, Applied Computational Chemistry, and Quantum Chemistry and Spectroscopy. Feedback from students and colleagues on her teaching work is excellent - she is a highly engaged and dedicated teacher. Over the past five years, Galia Madjarova has exceeded the required 360 hours of annual academic teaching hours, mostly lecturing to undergraduate and graduate students.

Assoc. Prof. G. Madjarova's scientific research is in the field of theoretical modeling using methods of computational chemistry of various systems: isolated molecules, polymers, complex colloidal systems, solid-phase materials with selective magnetic properties. These studies required the application of most diverse methods of computer modeling: quantum-chemical calculations, molecular dynamics, application of software for periodic calculations using density functional theory, modeling of interactions of biologically active ligands with bioreceptors. All this testifies that the candidate in the competition has excellent theoretical and practical methodical background in the field of the competition.

The scientific contributions in the published papers presented in the competition are in several directions, which I will consider sequentially.

- Using molecular dynamics calculations, the supramolecular structure of a mesophase containing glycerol monooleate (GMO), tricaprin and water was studied. The calculations showed that this complex system exists as a hexagonal structure, the result of various intermolecular interactions. This unexpected result illustrates very well the effectiveness of molecular dynamics as a method for studying the structure, possible transformations, and hence the functions of complex physicochemical systems / publ. 1,4/.
- The application of molecular dynamics simulations in examining the aggregation of bile acids in an environment well modeling the conditions in the human gastrointestinal tract is also very interesting. Essential factors contributing to aggregation, as well as the mechanisms related to these processes, have been revealed. This study illustrates very well the interest of Assoc. prof. Madjarova in studies related to processes in biological systems. The obtained results can be used in creating suitable methods and medicines for treatment of diseases.
- A central place in the studies of G. Madjarova is the creation of a suitable model of a neoplastic membrane, allowing the investigation of the mechanisms of interaction of antitumor agents with cancer cells /publ. 7-11/. An appropriate model was created to describe the processes of active transport of medicinal agents to the α -folate receptor. Molecular

dynamics simulations illustrated reliably the complex processes and mechanisms of delivery of biologically active compounds and their interaction with the respective bio receptors. In this series of studies, the focus was on processes of importance to both basic science and medicine. It can be emphasized that Associate Professor Madjarova does not hesitate to study very complex physicochemical and biological systems, regardless of difficulties in their theoretical modeling. The results obtained are impressive.

- Another important part of Prof. Madjarova's research is in the field of description and prediction of the properties of permanent magnets that do not contain rare earth elements /publ. 5.6/. These studies, together with a comprehensive literature review, are summarized in the monograph *Design of Novel Hard Magnetic Materials Without the Use of Rare Earth Elements*, ed. SU / publ. 12/. In these works, G. Madjarova shows skills of modeling of solid phase materials, another area in computational chemistry. In addition, the research also covers the development of a machine learning system aimed at predicting the magnetic properties of new materials based on prior known data, as well as information accumulated during the modeling process. The results obtained in this area are very comprehensive and illustrate the excellent potential of computational chemistry in characterizing complex solid-phase systems.

Prof. Galia Madjarova is a highly respected colleague at the Faculty of Chemistry and Pharmacy. She is engaged in administrative activities as the deputy dean for academic studies for the specialty "Pharmacy" and for postgraduate courses. She is a member of the FHF Faculty Council. She is chairpaerson of the ERducation council of the "Pharmacy" major, and also the head of the "Physical chemistry and molecular modeling" department for the "Chemistry" major. G. Madjarova is the co-head of the Laboratory for Modeling and Prediction of Processes and Properties of Materials for Clean Technologies at the Center of Excellence "National Center for Mechatronics and Clean Technologies". Galia Madjarova was the main driving force in the installation of a computer cluster at FHF. She is also the cluster administrator. Associate Professor Madjarova has played also a key role in the successful implementation of the Moodle system for online learning in the faculty. She has provided technical assistance to regular teachers and external lecturers in the use of the online learning system during the period 2020-2022.

Assoc. Dr. Galia Madjarova is a distinguished scientist with excellent international prestige in the field of computational and theoretical chemistry. The scientific results

presented above and their publication in leading scientific journals in the field /nine publications in journals from Q1 quartile of the list of 11 scientific articles presented in the competition/ underline the high level of her studies. The qualities of the candidate as a teacher and a very active participant in the organization and management of the academic work of the Faculty of Chemistry and Pharmacy emphasize her significant role in the overall activity of the Faculty.

All of the above gives me the reason to confidently recommend to the respected Scientific Council of the FHF to award the scientific title "Professor" in Professional Direction 4.2 Chemical Sciences (Theoretical Chemistry - Computational Chemistry), to Assoc. Dr. Galia Kostova Madjarova.

July 5, 2022

Reviewer: 
/Prof. Dsci. Boris Galabov/