

OPINION

of the materials, submitted for participation in a competition for the academic position "Professor" in a professional field 4.2. Chemical Sciences (Theoretical Chemistry - Computational Chemistry), published in the State Gazette, issue 21 of 15.03.2022 (p. 138) for the needs of the Faculty of Chemistry and Pharmacy (FCP) at Sofia University "St. Kliment Ohridski"

The only candidate in the competition is Associate Professor Dr. Galia Kostova Madjarova; Galia Madjarova; <https://orcid.org/0000-0002-6786-2719>; Author ID (Scopus): 6602638896; <https://www.researchgate.net/profile/Galia-Madjarova>; Web of Science ResearcherID: A-9124-2013

General characteristics of the received materials and the applicant. By Order № RD-38-169/28.03.2022 of the Rector of Sofia University, Prof. Anastas Gerdzhirov, I have been appointed as a member of the scientific jury for the present competition. The submitted materials by Dr. G. Madjarova for participation in the competition are in full compliance with the requirements of the Law for development of the academic staff in Republic of Bulgaria and the Regulations for its implementation, the Regulations on the terms and conditions for obtaining scientific degrees and occupation academic positions (AP) at Sofia University "St. Kl. Ohridski" (SU) and the Recommended Criteria of the FCP-SU for professional field (PF) 4.2. Chemical Sciences. Inspection of the above requirements for the AP "Professor" showed that the candidate fulfilled the required minimum of all indicators by groups **(A, C, D, E, F, G)** and collected **1009** points against the total required minimum of **760** points. There is no evidence and no reports of plagiarism have been received on the documents (scientific papers) submitted for the competition (Art. 26, par. 4).

Galia Madjarova was born on November 07, 1972. She graduated from FCP at SU in 1995 with Master's degree in "Chemical Physics and Theoretical Chemistry" and in 1999 she obtained the educational and scientific degree "Doctor" in PF 4.2. Chemical Sciences (Theoretical Chemistry). With a Ph.D. degree, the candidate fulfills the indicator "A" (**50 p.**). As a result of consistent career development in the field of theoretical chemistry, she holds the academic positions of Assistant, Chief Assistant and since 2013 she is an Associate Professor at the Department of Physical Chemistry, Laboratory of Quantum and Computational Chemistry of the FCP at SU, having accumulated 21 years of experience in the specialty. Assoc. Prof. Madjarova is registered in the Register of the academic staff in the Republic of Bulgaria, maintained by the National Centre for Information and Documentation (<https://ras.nacid.bg/dissertation-preview/16716>), where data on her academic degree (PhD) and academic position (Assoc. Prof.) are available. During her scientific career, the candidate carried out 9 specializations in Germany, UK, France and Japan. The project activity of the candidate is impressive: Assoc. Prof. Dr. Galia Madjarova has participated in 32 projects and presented scientific communications at 63 conferences and workshops. She has accumulated extensive administrative experience as a Deputy Dean for the academic activities; a member of the Faculty council of the FCP-SU, the General Assembly of the SU, the University academic committee of the SU; a head of the Department "Physical Chemistry and Molecular Modelling" for the specialty "Chemistry" and a chairman of the study council for the specialty "Pharmacy".

Research activities. Assoc. Prof. Dr. G. Madjarova is a co-author in **41** scientific papers, **31** of them are published in refereed and indexed journals in the **SCOPUS**/Web of Science database. At the time of writing, the total number of citations of the publications (excluding self-citations of all authors) is 339 and the h-index is 12 (SCOPUS).

In the current competition, Assoc. Prof. Madjarova participates with **one monograph** and **11 original research papers**, which exclude publications from her doctoral thesis and the competition for AP “Associate Professor” (2013). All papers are published in reputable international journals with high impact factor, e.g. *Journal of Chemical Theory and Computation* (IF ~6), *Journal of Molecular Liquids* (IF 5.1), *Physical Chemistry Chemical Physics* (IF 3.6), *The Journal of Physical Chemistry B* (IF 3.2) and they reflect in-depth research in the field of theoretical chemistry. The scientific works are with contributions to the modelling of the structures and properties of various systems using the methods of computational chemistry, correspond thematically to the scientific specialty "Theoretical Chemistry" of the competition and fully meet the requirements for the AP "Professor" according to the group of indicators "C" - **100 p.** for habilitation work - monograph (min. 100 p.) and "D" - **257 p.** for 9 publications in journals of category Q1, 1 - with Q2 and 1 - with Q4 (min. 220 p.).

Habilitation work. In fulfillment of the requirements of the competition for AP “Professor”, Assoc. Prof. Dr. Madjarova has submitted a habilitation work, entitled "***Design of novel hard magnetic materials without the use of rare earths***", including 92 pages. The magnetic characteristics and functional properties that determine the capacity of magnetic materials for industrial applications are analyzed in great depth. The worldwide need for the development of new hard-magnets using cheap and accessible raw materials, without rare earths (RE) and with a high recycling rates is outlined. The monograph contributes to the development of two theoretical approaches for modeling non-RE magnetic systems and calculating their magnetic characteristics as a means to predict new prospective magnets and guide their synthesis. With the help of spin-polarized DFT method and calculations of selected periodic hexagonal Fe_2YZ и Co_2XY (Y = Ni, Fe (Co), Pt; Z = Al, Ga, Ge, In, Sn) Heusler structures, correlations between magnetic moments, spin-orbit coupling of atoms in the three positions, total number of valence electrons, volume of the unit cell on the one hand, and total magnetic moment, saturation magnetization density (M_s), and magnetocrystalline anisotropy on the other are derived. Two hexagonal structures of Fe_2CoIn and Fe_2CoGa have been proposed as an alternative to magnetic materials with RE. The second approach, based on machine learning methods, is developed and validated for qualitative and semi-quantitative prediction of the total magnetic moment of the unit cell for an arbitrary structure from a given empirical formula and unit cell volume. The trained model enables rapid estimation of the magnetic moment of a large number of hypothetical systems and can effectively direct experimental and quantum chemical studies to the most promising systems.

It should be recognized that the research approach for theoretical characterization of the magnetism of metallic multicomponent periodic systems is not trivial due to consideration of spin-orbit coupling, spin polarization, the possible magnetic ordering, a sufficiently large grid of k-points, etc., calibration of the unit cell parameters and method validation. By accomplishing these tasks Assoc. Prof. Madjarova demonstrates a deep knowledge of solid state chemistry and magnetism, and skillful application of computational approaches to modeling magnetic periodic structures and machine learning.

Author's reference. Assoc. Prof. G. Madjarova has also presented a brief report on the scientific contributions of the publications included in the group of indicators "D". The author's reference is competently prepared and adequately reflects the scientific contributions of the candidate, as they can be divided into three main groups according to the type of systems studied:

- In eight papers (1, 4, 3, 7-11), the research is focused on modelling of biologically relevant structures – a biocarrier system (consists of glyceryl monooleate and water, in hexagonal mesophase), a stabilizing agent tricaprylin and entrapped lysozyme; aggregates of bile salts in aqueous solutions at physiological conditions; a drug transport system including a targeting ligand-carrier (folate or antifolate) and a folate receptor- α (FR- α) (as a drug target for cancer treatment). The computational results are invaluable in view of the possibility to explain the experimental data, to reveal the mechanisms of interaction between the components in the studied systems and to propose the optimal structures and conditions.
- Methodology study of the optical spectra for the molecular crystals and 1D polymer applying TDDFT "bootstrap kernel" formalism to compute the dielectric function and an estimation of the method's reliability (2).
- Modeling the magnetic properties of permanent magnets without RE in the structure. The study is focused on stable tetragonal and hexagonal Heusler compounds and an estimation of their magnetocrystalline anisotropy energies by calculating the spontaneous magnetization (5, 6).

For the purposes of the research, quantum chemical and molecular dynamic calculations are applied. It should be emphasized that the models and computational methods used are selected so as to reproduce the experimental systems and processes as much as possible.

In fulfillment of the minimum requirements for AP "Professor" (group of indicators **E** and **G**), the candidate reports scientometric data only on the papers presented for the competition: for group "**E**" – **172 p.** based on 86 citations (without self-citations of all authors), (min. 120 p.); for group "**F**" - **270 p.** for a leadership of 6 and a participation in 11 national projects, and membership in 2 international projects (min. 150 p.), for group "**G**" - **160 p.**, taking into account the h-index 12 (120 points), a new introduced course, supervision of 2 students (master's degree) and co-supervision of 2 students (bachelor's degree) (min. 120 p.). The educational and teaching activity of Assoc. Prof. Madjarova comprises the development and conduct of 6 lecture courses and 6 practical classes with annual academic employment between 598 and 931 hours.

In conclusion, the scientific contributions, publishing and teaching activity and participations in scientific projects of Assoc. Prof. Dr. G. Madjarova, prove that she is a highly qualified and reputable scientist in the field of theoretical chemistry, which fully corresponds to the scientific specialty "Theoretical Chemistry – Computational Chemistry" of the competition. After the analysis of the materials presented for the competition, **I find it reasonable to give my positive assessment by voting convincingly "yes" and recommend the Scientific Jury to propose to the Faculty Council of FCP at SU, Assoc. Prof. Dr. Galia Kostova Madjarova to be elected to the academic position "Professor" at the Faculty of Chemistry and Pharmacy, Sofia University in the professional field 4.2. Chemical Sciences, scientific specialty "Theoretical Chemistry-Computational Chemistry".**

20.07.2022
Sofia

Ivelina Georgieva, Prof. Dr.
Institute of General and Inorganic Chemistry-BAS