

OPINION

Concerning the competition for awarding the academic position of “**Professor**” in professional field 4.2. Chemical Sciences, scientific specialty “Physical Chemistry” pursuant to announcement in State Gazette No. 24 of March 21 2025

Candidate: **Assoc. Prof. Dr. Silvia Emilova Angelova**, Institute of Optical Materials and Technologies “Acad. Jordan Malinowski”, Bulgarian Academy of Sciences

Member of the Scientific Jury: Assoc. Prof. Dr. Tatyana Koutzarova, Institute of Electronics, Bulgarian Academy of Sciences

1. *General characteristic on the presented materials:* Assoc. Prof. Dr. Silvia Angelova, the sole candidate in the competition, graduated from the Faculty of Chemistry, St. Kliment Ohridski University of Sofia. She has acquired the educational-scientific degree of “doctor”, with thesis topic of “Calculated quantum chemical NMR parameters as a tool for studying tautomeric and conformational transformations”. At present, she holds the academic position of “Assoc. Prof.” in the Institute of Optical Materials and Technologies “Acad. Jordan Malinowski”, Bulgarian Academy of Sciences and is its Administrative - Scientific Secretary. Concerning Indicator C – habilitation work – scientific publications refereed and indexed in worldwide databases with scientific information – she participates in the competition with seven publications in refereed international journals with impact factor (Web of Science; Scopus), of which five fall into the Q1 quartile and 2, into the Q2 quartile. The points acquired under this Indicator are 165. Concerning Indicator D, 12 publications are presented in refereed international journals (Web of Science; Scopus), of which six falling in quartile Q1, four in quartile Q 2, one in quartile Q3 and 1 published in journal without SJR / IF. The sum of the points under this Indicator is 245. Concerning Indicator E11, 85 independent citations in 10 scientific publications are presented, pointing to the wide response within and recognition by the scientific community. Under this Indicator, the number of points is 170 (the minimum required being 120). Concerning Indicator F, Assoc. Prof. Dr. S. Angelova has submitted a list of the research projects of which she had been the Coordinator or a Research Team Member, together with the funding received (280 points). The number of points under all Indicators is in compliance with the minimal national requirements, the requirements of the Rules for Implementation of the Law on the Development of the Scientific Staff in Republic of Bulgaria, and exceeds the requirement for the minimum number points under the respective Indicators as stipulated in the Regulations on the conditions and procedures for acquiring scientific degrees and for occupying academic positions at the Institute of Optical Materials and Technologies “Acad. Jordan Malinowski”, Bulgarian Academy of Sciences.

2. *General characterization of the candidate's scientific and applied scientific activities:* Assoc. Prof. Dr. S. Angelova takes part in the competition in question with scientific contributions related to the field of Theoretical Chemistry. As evidenced by the submitted scientific papers, the contributions of Assoc. Prof. Dr. S. Angelova are on planning and performing theoretical calculations in view of studying the structure and properties of organic compounds and complexes, as well as interpreting the results obtained and their relationship with the experimental ones. The total number of her publications is 113; the number of the independent citations is 589 according to the Scopus database and the h-index 13. She is the Coordinator of a project funded by the Bulgarian National Science Fund. The administrative activities: Assoc. Prof. S. Angelova has been the Scientific Secretary of the Institute of Optical Materials and Technologies, BAS, since 2022. She had acted as a student mentor in the “Student Internship Programs” funded by the Ministry of Education and Science.

3. *Major scientific and/or applied scientific contributions:* The main scientific contributions in the publications presented instead of a habilitation thesis are related to applying quantum-chemical calculations for: studying the electronic structure and properties of chemosensory systems based on 1,8 - naphthalimide and rhodamine, as well as D-A⁺(D) chromophores for nonlinear optical applications; studying host-guest type complexes of dyes and cucurbit[7]uril. DFT and TD-DFT methods are used to study the geometry and electronic structure of 1,8-naphthalimide derivatives in order to explain the influence of different metal ions on the photophysical characteristics and the experimentally observed selective sensing ability. RhPzNH₂ is studied as a molecular logic device and is shown to act as a digital comparator. It is found that the interaction of the host molecule with the dye molecules can be predicted from a thermodynamic point of view using DFT calculations. New data are obtained useful in the design of supramolecular systems based on dyes and CB[7], which are relevant for photonics applications. New data on the electronic structure and properties of quinolinium chromophores are by DFT, HF and MP2 calculations. Based on theoretical and experimental studies, a strategy is proposed for the design of directly connected DA building blocks for the creation of new nonlinear optical materials on an organic basis. The scientific contributions in the publications under indicator D can be summarized as presenting a wide range of DFT functionals for quantum-chemical calculations in solving specific problems in isomerization, tautomerization, aggregation processes, optimization of the geometry of one or more molecules, etc.

The analysis of the submitted documents proves that the scientific works cited by the candidate constitute her personal contributions. These can be described as enriching the existing theoretical knowledge.

4. *Critical remarks and recommendations on the submitted works:* None

5. *Conclusions:* The review made of the scientific, applied scientific and scientific metrics indicators concerning the candidate demonstrate a full compliance with all applicable requirements – minimal national requirements pursuant to the Law on the Development of the Scientific Staff in Republic of Bulgaria and the Rules for its Implementation, to the minimal requirements of the Rules for the Conditions and Order of Acquiring Scientific Degrees and Holding Academic Positions in the Bulgarian Academy of Sciences, as well as to the Requirements for occupying academic position “Professor” at the Institute of Optical Materials and Technologies "Acad. Jordan Malinowski", Bulgarian Academy of Sciences. **All the above give me reasons to be deeply convicted in recommending the Scientific Jury to make a positive decision concerning Assoc. Prof. Dr. Silvia Emilova Angelova being awarded the academic position of “Professor” in professional field 4.2 “Chemical Sciences”, scientific specialty “Physical Chemistry”.**

Date 13.07.2025

Prepared by:

/Assoc. Prof. Dr. Tatyana Koutzarova/