

OPINION

on the competition for associate professor

4.2. Chemical Sciences (physical chemistry)

announced in the Official State Gazette, issue 41 of 21 May 2019.
candidate Assistant Prof. **Silvia Emilova Angelova PhD**

In the associate professor competition at the Institute for Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, there is one candidate is participating - Dr. Silvia Emilova Angelova. Silvia Angelova graduated from the Faculty of Chemistry at Sofia University "St. Kliment Ohridski" in 1995 obtaining Master degree in "Organic and Analytical Chemistry". In 2009 she defended her PhD in Theoretical Chemistry on the topic "Quantum-chemically calculated NMR parameters as a tool for study of tautomeric and conformational equilibria" at the Institute of Organic Chemistry with the Center of Phytochemistry at BAS. From 2000 to 2011, Silvia Angelova held a chemist position at the NMR Spectroscopy Laboratory and later a researcher in Computational Chemistry (substance construction, chemical thermodynamics and spectroscopy) at the same institute. Since 2011 she's been holding Assistant Professor Position.

The scientific activity of Dr. Silvia Emilova Angelova covers 62 scientific articles and 3 book chapters, 52 of them, published in international journals with an impact factor. The candidate participates in the competition with 28 publications divided according to the requirements of the law into two groups. According to the information provided by the candidate, those papers were cited 34 times. My check in Web of Knowledge and Scopus, with the exception of self-citations, returned almost the same results. Dr. Angelova has participated in both national and international projects. She has also participated in more than fifty national and international conferences.

Dr. Angelova's studies, included as publications in the current competition, focus mainly on applications of quantum-chemical calculations study of the structure and properties of molecular systems in the group of perylene, merocyanine, squarylium and croconium dyes and their potential application as photovoltaic solar cell, optoelectronics materials, or functional materials. Due to their hyperpolarizability and their solvatochromic properties, these dyes are of interest in applications where non-linear optical properties are required. The studies are aimed at both the search for classic calculations such as HOMO and LUMO orbit calculations and the differences between them, as well as a methodological development of DFT and TDDFT methods in terms of electron density transport, reorganization energy λ and coupling exciton energy. Applications of quantum-chemical calculations for studying the electronic structure in the ground state and excited state of tautomeric systems are also very interesting. Dr. Angelova has used calculations and has validated and clarified the mechanism of double proton transfer in an excited singlet state, which is a significant challenge for computational chemistry and has great practical application in areas such as photosensitization, sensory chemistry of metal complexes and laser dyes.

The scientific publications presented show that Sec. Dr. Angelova is an established scientist with a rich and varied professional experience, developing in an extremely interesting scientific field.

In conclusion, I believe that PhD, Assistant Professor Silvia Emilova Angelova meets all the requirements of the law for occupying the academic position of Associate Professor. She is a specialist in quantum computing, theoretical chemistry and computational chemistry. Based on the above, I propose Ch. Prof. Dr. Silvia Emilova Angelova to be elected Assistant Professor at the Institute of Optical Materials and Technologies "Acad. J. Malinowski" at the Bulgarian Academy of Sciences.

Sofia,

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Having prepared the opinion:

Assoc. Prof. Dr. Veselin Petrov