**Attn.**
**Head of the Scientific Jury,**
**appointed by order № РД-15-305/14.05.2025**
**issued by the Director of IOMT, BAS**

***I present:*** REVIEW
on competition for academic position **professor** in a professional direction 4.2. Chemical sciences, scientific field "Physical chemistry", announced in SG, no. 24 / 21.03.2025.

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# REVIEW

on competition for academic position **professor** in a professional direction 4.2. Chemical sciences, scientific field "Physical chemistry", announced in SG, no. 24 / 21.03.2025.

candidate **Assoc. Prof. Silvia Angelova**, IOMT, BAS.

Reviewer: Prof. Bogdan Ranguelov, IPC, BAS

One candidate only participates in this competition, namely Assoc. Prof. Silvia Angelova, PhD. The presented materials for participation in the competition procedure are complete, very well structured and collected, described in details with attached evidence materials and in accordance with the National requirements and the Rules for Academic Development in IOMT, BAS, thus allow evaluation of the candidate participating in the competition.

## I. Short bio and analysis of the career profile of the candidate

Silvia Angelova graduated with a higher education degree from the Faculty of Chemistry at Sofia University "St. Kliment Ohridski" in Sofia in 1995, majoring in Chemistry. Concurrently, she completed a postgraduate qualification in "Business Management and Marketing" at the Institute for Postgraduate Studies at the University of National and World Economy in Sofia. In 2001, she began working at the Institute of Organic Chemistry with a Center for Phytochemistry at the Bulgarian Academy of Sciences (BAS), where, in 2009, she earned a PhD degree through the Higher Attestation Commission (VAK) in the professional field 4.2. Chemical Sciences, specializing in Theoretical Chemistry. The title of her dissertation was "Quantum-Chemically Calculated NMR Parameters as a Tool for Studying Tautomeric and Conformational Transformations." In her work, quantum-chemical calculations were used to determine the relative energies of different tautomers and conformers, aiding in the identification of the most stable forms and understanding which transformations are thermodynamically favorable. From 2005 to 2011, she held positions as a Research Associate, Assistant, and Chief Assistant at the Institute of Organic Chemistry with a Center for Phytochemistry, BAS. Between 2012 and 2023, she pursued a postdoctoral specialization at the University of Alcalá (UAH) in Alcalá de Henares, Madrid. Since 2019, she has been an Associate Professor at the Institute of Optical Materials and Technologies "Acad. Jordan Malinowski," BAS, and since 2022, she has also served as the Scientific Secretary of the institute.

## II. General description of the presented data materials

Assoc. Prof. Dr. Silvia Angelova has submitted all required documents and corresponding evidence in accordance with the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria (ZRASRB) and the Regulations of the Institute of Optical Materials and Technologies (IOMT) for the implementation of ZRASRB. These include: a curriculum vitae, a PhD diploma, a list of articles for the habilitation work, a list of publications, a list of citations and reviews, a list of participations in international and national projects, a report on original scientific contributions, summaries and copies of publications, and other relevant materials. The materials submitted for the competition are complete, very well-structured, appropriately color-illustrated, clearly organized, and thoroughly described with attached supporting evidence.

In the competition for the academic position of "Professor," Assoc. Prof. Angelova participates with publications grouped into two categories (in accordance with the requirements of the Regulations for the Implementation of the Law on the Development of the Academic Staff in the Republic of Bulgaria (ZRASRB) for the procedure for occupying the academic position of "Associate Professor" or "Professor," with a formula for equating a monograph to an equivalent number of

articles):

**First Group:**
These are scientific publications equated to a habilitation work (group of indicators "B," indicator "4"): seven in total (numbered in the candidate's full list of articles as 68, 69, 84, 85, 97, 100, 104). Of these publications, five are in Q1 journals and two are in Q2 journals.

**Second Group:**
These are scientific publications (group of indicators "G," indicator "7"): twelve in total (numbered in the candidate's full list of articles as 15, 19, 40, 43, 58–60, 70, 73, 75, 105, 109). Of these publications, six are in Q1 journals, four in Q2 journals, one in a Q3 journal, and one is indexed without JCR or SJR.
The high number of Q1 and Q2 publications indicates the candidate's involvement and contributions within strong research teams, highly regarded by the international scientific community. This suggests that the candidate is part of groups producing scientifically significant and innovative research, which receives broad support and recognition.

The total number of publications by Assoc. Prof. Angelova is 113 (one hundred and thirteen). Notably, 50 (fifty) of these were published in the period from 2020 to 2025 (a five-year period, i.e., after assuming the academic position of "Associate Professor" at IOMT at the end of 2019), corresponding to numbers 64–113 in the overall list of publications.

Silvia Angelova leads a specialized course at the BAS Training Center titled "Computer Modeling of Molecular Structure and Optical Properties of Single Molecules and Supramolecular Aggregates."

A very positive impression is made by the number of graduates who have defended their bachelor's or master's theses under the supervision or co-supervision of Assoc. Prof. Angelova—a total of fifteen, primarily from Sofia University. Among these graduates, some have subsequently pursued PhD studies within the BAS system, including one who is a recipient of the National Award "13 Centuries Bulgaria" for Young Talents in Contemporary Art and Science in 2022.

**III. Evaluation of the general scientific activity and overall academic career**

The overall scientific activity of Assoc. Prof. Dr. Angelova is in the field of computational chemistry, with the articles submitted for the competition reflecting various aspects of scientific research on dyes and systems containing chromophore groups, primarily using computational chemistry methods, mainly DFT and ab initio. Quantum-chemical calculations based on DFT are powerful tools for studying dyes and systems with chromophore groups. They provide fundamental insights into the electronic structure and properties of these systems, which are essential for the development of new and improved materials with diverse applications in science and technology.

The main scientific contributions in the publications submitted in lieu of a habilitation monograph can be thematically grouped into three main categories, resulting from the application of quantum-chemical calculations to study the structure and properties of molecular systems:

**I)** Application of quantum-chemical calculations to study the ground-state electronic structure and properties of chemosensor systems based on 1,8-naphthalimides and rhodamines [68, 69, 84, 97, 100]:

Chemosensor systems based on 1,8-naphthalimides and rhodamines are of great interest due to their ability to respond to various external stimuli such as pH, metal ions, and biomolecules. DFT-based quantum-chemical calculations provide valuable information about the ground-state electronic

structure of these systems. By calculating electron densities, orbitals, and energy levels, the mechanisms of sensor responses can be understood, and the sensitivity and selectivity of the systems can be predicted. This enables the rational design of new and improved chemosensors with enhanced efficiency and specificity.

**II)** Application of quantum-chemical calculations to study host-guest complexes of dyes and cucurbit[7]uril [104]:

Host-guest complexes formed between dyes and cucurbit[7]uril are of interest due to their unique photophysical and photochemical properties. Cucurbit[7]uril, with its cavity, can encapsulate various dyes, altering their spectral and fluorescent characteristics. DFT-based quantum-chemical calculations allow detailed investigation of the electronic structure and interactions in these complexes. This knowledge is crucial for the development of new materials for optical devices, sensors, and biomedical applications.

**III)** Application of quantum-chemical calculations to study the ground-state electronic structure and properties of D-A+(D) chromophores for nonlinear optical applications [85]:

D-A+(D) chromophores, where D represents a donor, A an acceptor, and + symbolizes the repetition of the donor group, are promising candidates for nonlinear optical materials. Nonlinear optical properties, such as two-photon absorption and second-harmonic generation, are essential for communication technologies and information processing. DFT-based quantum-chemical calculations provide detailed information about the electronic structure and energy levels of these chromophores. By calculating electron densities and orbitals, the nonlinear optical properties of systems can be predicted and optimized for applications in telecommunications, medicine, and military technology.

Regarding the scientific publications under group indicator "G," indicator 7, all 12 publications pertain to the application of computational methods to study the structure and properties of organic compounds and complexes. These publications illustrate a wide range of scientific problems addressed using computational methods (independently or in combination with experimental approaches).

## IV. Evaluation of the main scientific contributions

The main scientific contributions and results of Assoc. Prof. Angelova are of a fundamental nature.

IV. 1. Regarding the scientific contributions in the seven publications submitted in lieu of a habilitation monograph:

IV. 1. 1. Application of quantum-chemical calculations to study the ground-state electronic structure and properties of chemosensor systems based on 1,8-naphthalimides and rhodamines.

This includes the articles numbered 68, 69, 84, 97, and 100.

With the aid of quantum-chemical calculations (classical Density Functional Theory and Time-Dependent Density Functional Theory), data on the structure of dyes, derivatives of 1,8-naphthalimide, have been obtained. These are quantum-mechanical methods for studying the electronic structure and dynamics of molecules and materials, particularly in the case of excited states. Density Functional Theory has been extended to time-dependent systems, enabling the calculation of properties such as absorption spectra, electronic transitions, and responses to external fields. This is a commonly used method for calculating UV-Vis spectra, excited-state energies, and

photochemical processes in chemistry, physics, and materials science.

Dyes derived from 1,8-naphthalimide are a class of organic compounds used as fluorescent dyes and pigments due to their excellent optical properties, such as high fluorescence, photostability, and vibrant colors. They are based on the 1,8-naphthalimide structure, which consists of a fused aromatic system comprising a naphthalene ring with an imide group at positions 1 and 8. These compounds find applications in various fields, including the textile industry, sensors, biomedical research, and optoelectronics. These dyes typically exhibit strong fluorescence in the ultraviolet (UV) or visible spectrum, often in the yellow-green or blue-green range. The wavelength of absorption and emission can be tuned by modifying the substituents on the naphthalimide structure, making them suitable for specific applications.

Derivatives of 1,8-naphthalimide have been investigated as sensor systems for detecting cations, anions, or neutral analytes, which are major industrial environmental pollutants. For two new 1,8-naphthalimide derivatives, calculations using DFT and TDDFT methods were performed, enabling the study of the geometry and electronic structure of these systems. This included examining the influence of various organic solvents on absorption spectra, protonation, and the ability of these systems to form complexes with metal cations, aiming to explain the impact of different metal ions on the photophysical properties of the studied systems. Another 1,8-naphthalimide derivative was investigated as a sensor for mercury ions. In the context of sensors for mercury ions ($Hg^{2+}$), these compounds are studied for their ability to selectively recognize and detect the presence of these toxic ions in various media, such as water, biological samples, or industrial waste. These sensors often exhibit low detection limits (in the nanomolar or even picomolar range), making them suitable for monitoring mercury in the environment, where its concentrations are low but toxic. The interaction between the sensor and $Hg^{2+}$ typically leads to a change in the electronic structure of the naphthalimide, which can manifest as: i) fluorescence enhancement ("turn-on" effect) through chelation (binding) of mercury, which prevents quenching processes; ii) fluorescence quenching ("turn-off" effect) due to energy or electron transfer between mercury and the fluorophore; iii) a shift in the emission wavelength, enabling visual detection (color change). This work is significant because designing 1,8-naphthalimide derivatives requires careful consideration to achieve a balance between selectivity, sensitivity, and solubility in aqueous environments. Additionally, some sensors may also respond to other heavy metal ions (e.g., $Ag^{+}$, $Cd^{2+}$), necessitating further optimization.

New fluorescent dendrimers, obtained by incorporating 1,8-naphthalimides into polypropyleneamine (PPA) and polyamidoamine (PAMAM) dendrimers through so-called peripheral modification, have been investigated. These are innovative macromolecules with a tree-like structure that find applications in fields such as sensors, optoelectronics, and biomedicine due to their unique optical properties.

A fragment of the system was modeled, for which the geometry in the ground state was optimized, and possible interactions with explicit solvent molecules (methanol) were examined, as hydrogen bonds with solvent molecules are crucial for the 3D structure of the dendrimer. Preferred protonation sites were identified, and UV spectra were theoretically predicted. The compounds were investigated for antimicrobial and cytotoxic activity in their free state and after being applied to the surface of cotton fabric. The dendrimer exhibited slightly lower activity compared to its monomeric analog but was found to be significantly less cytotoxic. The dendrimer applied to cotton fabric prevented the formation of bacterial biofilm on the fabric surface.

Rhodamine is a family of organic compounds known as xanthene dyes, characterized by bright fluorescence and high photostability. They are widely used in biology, chemistry, and industry due to their ability to emit light when excited at specific wavelengths.

Rhodamines can exist in two forms:

i) A non-fluorescent form, in which the molecule does not emit light when irradiated with a specific wavelength. This is typically due to a closed chemical structure that suppresses fluorescence.
ii) A fluorescent form (open form): Under certain conditions (e.g., changes in pH, binding to ions or molecules), the molecule transitions to a structure that allows light emission (fluorescence). This interconversion (reversible switching between the two forms) is a key feature of rhodamines and is utilized in sensors, as it enables the "on" or "off" switching of fluorescence depending on external stimuli (e.g., the presence of metal ions).

A hybrid compound (RhPzNH2), combining rhodamine and pyrazole, was investigated and designed as a chemosensor for $Cu^{2+}$ ions. Through simulations, its structures and interactions with metal ions at various ratios were studied. The lack of experimental data necessitated the use of computational simulations. The compound shows potential as a molecular logic device, functioning as a digital comparator, making it interesting for applications in sensors and molecular electronics (the compound can "signal" through fluorescence when bound to a metal ion, rendering it suitable for molecular electronics or sensors).

IV. 1. 2. Application of quantum-chemical calculations to study host-guest complexes of dyes and cucurbit[7]uril.
This includes the article numbered 104.

Cucurbit[7]uril (CB[7]) is a macrocyclic molecule from the cucurbituril family, used in supramolecular chemistry as a "host" for forming host-guest complexes. The specific structure of this molecule, particularly the presence of a "cavity" in its internal space, imparts several interesting properties, such as: the ability to encapsulate hydrophobic or aromatic molecules, such as dyes or drugs; facilitated binding with cationic or polar molecules through ion-dipole and hydrogen bonds; good water solubility; and the formation of stable complexes, especially with cationic molecules like dyes (e.g., methylene blue, rhodamine B).

Applications of CB[7] primarily include sensors, where it modifies the optical properties of dyes for analytical purposes; drug delivery, where it is used for encapsulation and controlled release of active substances; photocatalysis and stabilization; and the textile industry, where it enhances the durability of dyes.

However, in solid matrices (e.g., polymeric materials), dyes used for fluorescence exhibit reduced efficiency. This limits their applications in technologies reliant on fluorescence, such as sensors or optical devices. The main issues are low fluorescent quantum yield and poor photostability, i.e., the dye's resistance to degradation under light exposure.

When CB[7] is added to a copolymer hydrogel (a flexible polymeric material capable of retaining water, with covalently bound rhodamine B dye molecules), it is known to increase the fluorescent quantum yield from 17% to 51% and improve photostability by 15-fold, making the dye significantly more resistant to degradation. This forms the basis for studies involving the modeling of host-guest complexes for a series of laser dyes (Pyridine 1, Pyridine 2, Rhodamine 6G, Rhodamine B, and Rhodamine 700) with the same host system, CB[7], to evaluate CB[7]'s ability to encapsulate these structurally diverse dyes within its cavity. The process was investigated in the gas phase and with consideration of environmental effects, using explicit solvents chloroform and dimethyl sulfoxide. The interaction between the host molecule and the dye molecules was predicted, affecting their photophysical properties, primarily enhancing their photostability. Additionally, confining dye molecules within the CB[7] cavity is likely to reduce non-radiative decay pathways, leading to an increase in fluorescent quantum yield. These effects make CB[7] an attractive encapsulating agent for applications in laser technologies and other photonic devices requiring stable and highly fluorescent materials.

As a result of this entirely theoretical study, valuable new structural data were obtained, and guidelines were outlined for designing supramolecular systems based on dyes and CB[7], which have potential applications in rapidly developing fields such as photonics and materials science.

IV. 1. 3. Application of quantum-chemical calculations to study the ground-state electronic structure and properties of D-A+(D) chromophores for nonlinear optical applications.
This includes the article numbered 85.

New chemical compounds, referred to as D-A+ chromophores, synthesized via the Stille reaction—an organic chemical reaction used to couple two carbon atoms by forming a new carbon-carbon bond—were investigated. This reaction is particularly useful in the synthesis of complex organic molecules, as it enables efficient coupling of various functional groups with a high degree of tolerance toward other functional groups in the molecule. Chromophores are molecules with potential applications in nonlinear optics, such as in lasers or sensors. These chromophores are compounds that absorb and emit light and, in this case, consist of: i) an acceptor part (A+)—quinolizinium cations (positively charged molecular fragments), and ii) a donor part (D)—N-heterocycles rich in π-electrons, i.e., molecules that readily "donate" electrons. Typically, chromophores feature a so-called "conjugated system" (a long chain of bonds facilitating electron movement between the donor and acceptor). However, in this case, the donor and acceptor are "directly connected" without a conjugated system. This novel approach demonstrates promising nonlinear optical properties. This method enables the straightforward creation of "one-dimensional (D-A+)" and "two-dimensional (D-A+-D)" chromophores. These molecules can serve as alternatives to traditional chromophores for applications in nonlinear optics and organic optical materials.

The molecules were experimentally studied, with measurements of hyperpolarizability β, which indicates how strongly the molecules respond to an electric field—a key property for nonlinear optical applications. Hyperpolarizability β is a physical quantity that describes the nonlinear optical response of a material or molecule to an external electric field. It characterizes the system's ability to generate second harmonic generation (SHG) or other nonlinear optical effects, such as the electro-optic effect.

The theoretical investigation employed computational methods to analyze the electronic structure, linear and nonlinear optical properties, HOMO and LUMO orbitals, and their energy gap, which determines the optical properties. The influence of "substituents" (chemical groups added to the molecule) on these properties was also examined. The computational methods used include:
i) HF (Hartree-Fock) - a fundamental method based on the mean-field approximation, where electrons are considered to move in an averaged field of other electrons;
ii) DFT (Density Functional Theory) - which uses electron density instead of the wave function to calculate energy;
iii) MP2 (Møller-Plesset Perturbation Theory, second order) - a post-HF method that incorporates corrections for electron correlation using perturbation theory.

As a result, the combined experimental and theoretical investigation has enabled the proposal of a "new strategy" for designing chromophores with a direct donor-acceptor connection, which could lead to the development of new, more efficient, and easier-to-produce materials for nonlinear optics.

IV. 2. Regarding the scientific contributions in the twelve publications under group indicator "G," indicator 7:

All twelve publications in this group focus on the use of computational methods to analyze the structure and properties of organic compounds and complexes. They are selected to demonstrate a

variety of scientific problems addressed through computational techniques, either independently or in combination with experimental data. A wide range of DFT functionals was employed. The studies cover processes such as isomerization (a process in which one molecule transforms into another molecule with the same molecular formula but a different structural configuration), tautomerization (a specific type of isomerization in which a hydrogen atom migrates from one atom to another within the same molecule), aggregation, formation of complexes with metal cations, water molecules, and others, as well as homolytic cleavage of the O-H bond (a process in which the covalent bond between an oxygen (O) and hydrogen (H) atom breaks evenly, with each atom receiving one electron from the shared electron pair, typically occurring in reactions at high temperatures or under the influence of light (photolysis)). I will focus only on a specific subset of these studies.

Part of the studies are related to hydrazones (derivatives of hydrazine and ketones or aldehydes) as functional materials, focusing on their application as rotational switches and the use of computational methods to analyze their properties. By modifying functional groups (e.g., phenyl, naphthyl, quinolinyl), the optical, electronic, or mechanical characteristics of hydrazones can be "tuned."

Computational methods such as PCM (Polarizable Continuum Model) and SMD (Solvation Model based on Density) were used to model the effects of solvents on molecular properties. These methods are particularly useful for studying systems like hydrazones in solution, where the solvent influences energies, geometries, and optical properties. PCM models the solvent as a continuous medium with a specific dielectric constant surrounding the molecule, which is placed in a "cavity" (typically spherical or shaped to follow the molecular contour), treating the solvent as a polarizable continuum. SMD, an advanced solvation model developed by Truhlar and collaborators, combines the continuum approach of PCM with additional parameters (e.g., surface tension, hydrogen bonds) for a more accurate description of the solvent. It is preferred for complex systems where hydrogen bonds or dispersion effects are significant (e.g., hydrazones in polar solvents). Both models are combined with methods such as HF, DFT, or MP2 to study molecular properties. SMD is particularly useful when hydrazones form hydrogen bonds with the solvent or are studied in mixed solvents. The use of PCM or SMD with DFT (e.g., B3LYP) or MP2 enables accurate modeling of the on/off state energies of hydrazone switches in solution.

The potential of dietary supplements and functional foods as alternative therapies for the treatment of (pre)hypertension was investigated, focusing on bioactive peptides derived from food. Dietary supplements and functional foods are products containing bioactive compounds capable of positively impacting health, including regulating blood pressure in (pre)hypertension (high blood pressure or prehypertensive conditions). Bioactive peptides are short chains of amino acids that can mimic or modulate physiological processes in the body, such as blood pressure regulation. Val-Pro-Pro (VPP) is a tripeptide (consisting of three amino acids: valine, proline, proline), derived from dairy products, typically through fermentation or enzymatic processing of casein. It is studied for its presumed ability to inhibit angiotensin-converting enzyme (ACE), which plays a key role in blood pressure regulation. ACE converts angiotensin I into angiotensin II, which constricts blood vessels and increases blood pressure. Inhibiting ACE can reduce this pressure. The study compares the VPP tripeptide with two pharmaceutical ACE inhibitors: captopril and lisinopril, which are standard drugs for treating hypertension. The focus is on the interaction of these compounds with the active site of ACE—the key structural-functional element of the enzyme, where the zinc ion ($Zn^{2+}$) plays a role in catalytic activity. Captopril and lisinopril exhibit high affinity for the ACE

active site, meaning they bind strongly and effectively inhibit the enzyme, explaining their efficacy as drugs. VPP has a lower affinity for the ACE active site, suggesting its inhibitory activity is weaker compared to pharmaceutical drugs. The study elucidates the thermodynamic aspects (energy characteristics such as bond stability and binding energy) of the coordination between inhibitors and the ACE active site. VPP may have potential as a natural alternative for blood pressure regulation, but its effectiveness is lower than that of synthetic drugs like captopril and lisinopril. This suggests that functional foods containing VPP (e.g., fermented dairy products like certain types of yogurt) can contribute to the prevention or maintenance of normal blood pressure but are not a substitute for pharmaceutical treatments in severe hypertension. The results highlight the importance of molecular design and understanding interactions at the atomic level for developing new therapeutic approaches. The study shows that VPP has potential as a bioactive peptide for supporting cardiovascular health, but its effectiveness is limited compared to pharmaceutical ACE inhibitors, emphasizing the role of functional foods as a complementary, rather than primary, therapy for hypertension.

A study was conducted on oxidative stress, lipid peroxidation, and the antioxidant activity of phenolic compounds, with an emphasis on the relationship between their chemical structure and functionality. Oxidative stress is a condition characterized by an imbalance between the production of reactive oxygen species (ROS) (e.g., free radicals such as hydroxyl radical •OH or superoxide anion $O_2^-$) and the body's ability to neutralize them through antioxidant systems (enzymatic, such as superoxide dismutase, or non-enzymatic, such as vitamins C or E). Lipid peroxidation is a process in which ROS attack unsaturated fatty acids in lipid membranes, leading to radical chain reactions. This disrupts membrane integrity and results in the accumulation of products such as peroxides, aldehydes, and acids, which serve as markers of oxidative stress. Lipid peroxidation is a key pathological process in diseases such as atherosclerosis, neurodegenerative disorders, and cancer.

Forty phenolic antioxidants, including natural (e.g., polyphenols found in plants) and nature-inspired (synthetic analogs) compounds, were studied, with nine being newly synthesized. The aim was to analyze their antioxidant activity and role as modulators of oxidative stress, focusing on the structure-activity relationship. Theoretical methods such as DFT were used to analyze the electronic structure, energy characteristics, and reactivity of the molecules, while (Q)SAR was employed to predict antioxidant activity based on the chemical structure of the compounds. The kinetics of uninhibited and inhibited lipid oxidation, as well as the transformation of antioxidants during oxidative stress, were analyzed. Particular attention was given to the initial reactions leading to radical formation, a key stage in lipid peroxidation. It was shown that the position and nature of substituents (e.g., hydroxyl or methoxy groups) influence the ability of phenols to donate electrons or hydrogen atoms, which is critical for their antioxidant activity. It was demonstrated that antioxidant efficacy depends on their concentration, with higher concentrations generally enhancing oxidation inhibition, though optimal levels exist beyond which the effect diminishes. The (Q)SAR analysis indicates that specific structural features (e.g., the number and position of OH groups, electron delocalization) correlate with higher antioxidant activity. Overall, the combination of DFT and (Q)SAR enables the prediction of antioxidant activity without the need for extensive experiments, accelerating the development of new compounds.

The study provides valuable insights into the antioxidant activity of phenolic compounds and their role in counteracting oxidative stress by inhibiting lipid peroxidation. Through a combination of experimental (auto-oxidation, chemiluminescence) and theoretical (DFT, (Q)SAR) methods, the

relationship between the chemical structure of phenols and their efficacy was established. The results underscore the importance of hydroxyl and methoxy groups, as well as the influence of concentration and substitution on antioxidant properties. This research can support the development of new antioxidants for medical, food, and cosmetic applications.

Of the 19 publications (7+12) submitted for the competition, the candidate is the first author of 4 publications [19, 40, 58, 109], the last (leading) author of 3 publications [70, 104, 105], the corresponding author of 8 publications [19, 58, 59, 60, 70, 73, 75], and 1 publication is single-authored [59].

### V. Citataions

From the presented reference regarding the observed citations of the candidate, it is evident that the publications for participation in the competition (group indicators "B", indicator 4) are well received in scientific circles and have been cited shortly after their publication. At the time of preparing this reference, 31 citations of articles under group indicators "B", indicator 4, and 54 citations of articles under group indicators "G", indicator 7, have been observed.

### VI. Critics and suggestions

Overall, I do not have any critical remarks about the candidate's work and am pleased to use this opportunity to provide a recommendation that can be beneficial both to him and all researchers working in the field of theoretical and simulation studies. Modern science in this area is developing at an extremely rapid pace, thanks to the continuous improvement of computational methods and the introduction of innovative technologies. Among them, special attention should be paid to advancements in machine learning, neural networks, and applications of artificial intelligence. These tools not only expand the possibilities for analysis and modeling of complex systems but also offer new approaches to solving problems that were previously difficult to resolve. I recommend that the candidate continue to develop his skills towards integrating modern computational techniques while maintaining a high standard in his research. This will allow him to remain competitive and make significant contributions to the progress in the field of theoretical and simulation studies.

## OVERALL DECISION

Based on overall evaluation of the presented materials, I give my categorically positive opinion and strongly recommend the members of the Scientific Jury to award Dr. Silvia Angelova the academic position of "**professor**" in professional direction 4.2. Chemical sciences, scientific field "Physical chemistry".

04/07/2025 This review is prepared by:

Prof. Bogdan Ranguelov