OPINION

by Prof. Petko Marinov Ivanov

in accordance with the materials presented in a competition for an academic position "**ASSOCIATE PROFESSOR**", direction 4.2. Chemical Sciences (Theoretical Chemistry), published in the State Gazette, issue 63 of 30.07.2021.

The only candidate participating in the competition is **Assist. Prof. Dr. Julia Ruslanova Romanova.**

Grounds for preparing the opinion: Order RD-38-455 / 21.09.2021 of the Rector of Sofia University "St. Kliment Ohridski ".

1. General information about the candidate

Assist. Prof. Dr. Julia Ruslanova Romanova was born on March 19, 1983 in the town of Shumen. She graduated from the High School of Natural Sciences and Mathematics in the same city in 2001. She obtained a bachelor's degree in Chemistry in 2005 and a master's degree in Chemistry, professional qualification "Computational Chemistry" in 2006 at Sofia University "St. Kliment Ohridski". After conducting research at Sofia University and the University of Haute-Alsace, France, in 2010 she defended her dissertation on "Influence of the environment on the geometry, electronic structure and magnetic properties of polyaniline" to acquire the educational and scientific degree "Doctor" in the scientific specialty "Theoretical Chemistry". As a natural continuation of the research in her dissertation, the following year she completed a 6-month postdoctoral fellowship at FCP-SU and a 3-month specialization at the Leibniz Institute of Polymers in Dresden, Germany. 2012-2014 - postdoctoral fellowship at the University of Namur, Belgium, with the topic "Simulation of vibrational and resonance Raman spectra of viologens (DFT and CASSCF/CASPT2 calculations)". Research Fellow 2014-2016 at the Institute for Leading Technologies at the University of Surrey, UK. Using computational methods, she examined some metal polymers and organometallic complexes sensitive to external stimulation. After a two-year maternity break, since 2018 she acquired the position of Assist. Prof. in the Department of Inorganic Chemistry at the Faculty of Chemistry and Pharmacy at Sofia University.

2. Scientific publications of the candidate

The candidate is a co-author of 24 scientific publications indexed in Scopus, 4 chapters from books (1 of them indexed in Scopus, 2 in Web of Knowledge), 2 articles in conference proceedings and one patent. Participates in the competition with 14 scientific publications and one chapter of a book. 9 of the publications are in journals with rank Q1. Three of the scientific publications are in *J.Phys.Chem. (C)*, 1 publication in *Angew.Chem.Int.Ed*., *J.Phys.Chem.Letters*, *Chemistry-European Journal*, *PhysChemChem- Phys*, *Eur.J.Inorgan.Chem*. In 6 of the scientific communications she is the first author (with main contribution in conducting the quantum chemical calculations and analysis of the results), and in 5 publications - corresponding author (with main contribution in the problem setting, methodology and analysis of the results). Six of the publications are from the last 5 years (3 (Q1), 3 (Q2)). There are 24 participations with reports at conferences. Guest Editor of a Special Issue of *Molecules-MDPI* "Metal-Organic Complexes: Applications in Chemistry and

Materials Science". "Reference with selected citations" for 3 Q1-publications (53 citations) is presented. The total number of citations of all publications of the candidate is 249. h-index 11. I have absolutely no doubts about the candidate's contribution to the publications submitted for the competition. The documents for participation in the competition are prepared precisely and intelligently.

3. Participation in research and applied projects

Evidence for participation in 2 current projects financed by NSF and NSF-SU is presented, and the candidate is the leader of the latter. 25 is the total number of research projects in Bulgaria and abroad in the development of which Dr. Romanova has participated since 2004.

4. Study employment and scientific guidance

During the previous three academic years the candidate has 222, 413 and 295 hours of classroom employment, related to the management of the preparation by the students (1st year Chemistry) of 11 course works (2 of them research). In the framework of scientific projects, Assist. Prof. Dr. Romanova supervised the work of one doctoral student and 4 research students. Scientific consultant for 1 bachelor's thesis and 1 doctoral dissertation.

5. Scientific contributions

The scientific contributions of Assistant Professor Dr. Julia Romanova are in the field of applied computational chemistry and are grouped by her in three areas: (1) Organic molecules with open electron shell (4 Q1 publications) - Research conducted in partnership with 6 research groups from countries in Europe; (2) Organometallic complexes (3 Q1 publications) - Research mainly on postdoctoral issues in Surrey-UK (works 6, 7, 9, 15) and successfully continued in FCP-SU (works 3 and 5); (3) Theoretical spectroscopy (2 Q1 publications) - Research conducted during postdoctoral studies in Belgium.

5.1. Organic molecules with open electron shell

It has been shown that the electromotive force (open-circuit voltage, V_{oc}) in a in single-layer photovoltaic cells containing the emeraldine salt as a photoactive component can be significantly affected by the polarity of the solvent [12]. It has been established diradical character of the monomers and the dimeric intermediates in the radical polymerization of poly-*p*-phenylene vinylene by the method of Gilch (CASSCF / CASPT2 calculations) [8]. The stability and the optical properties of boron-dopped polycyclic chromophores (anthrecenes and phenanthrenes) have been explained and new chromophores for singlet fission have been proposed [4]. A review article presents an overview of molecular design strategies for singlet fission chromophores, focusing on the significant contributions of female researchers in the field [2]. By combining quantum chemical reactivity indices and chemometric approaches, an approach has been proposed to predict the laboratory stability of organic molecules, and thus the potential for the design of stable materials with photovoltaic properties. It has been demonstrated that molecules of a non-zero diradical character can also be laboratory stable [1].

5.2. Organometallic complexes

Studies on organometallic complexes involving Cu(II), Pt(II), Pd(II), Ru(II) and Au(I) have been performed. Rules for the molecular design of spin-hybrid molecular magnets based on orbital overlap between metal and ligand have been proposed [14]. The factors influencing the enhancement of the metallophilic interactions in the ground state and the role of the ligand

field for the metallophilic interactions in the excited state of Pt(II) complexes have been clarified. It has been found that the replacement of Pt(II) with Pd(II) in organometallic complexes prevents the intermolecular interactions in the excited state. The concentration and phase dependent luminescent properties of Pt(II) complexes are explained by the formation of excimers with a dominant metallophilic interaction [7, 9, 15]. New luminophores with the possibility of radiation in two different energy ranges based on heteroleptic complexes of Ru(II) [6] have been proposed, in particular new pH-sensitive luminescent materials [5]. An explanation for the cytotoxicity of Au(I) complexes has been proposed, as it has been shown to depend on the σ-donor properties of the isolated ligands [3].

5.3. Theoretical spectroscopy

The resonance Raman and UV/vis absorption spectra of methyl viologens and paraphenylene-extended viologens were simulated by multiconfiguration method (SS)-, (SA), (SA2)-CASSCF) and the hybrid exchange-correlation functional LC-BLYP with different range-separating parameters. It has been shown that the electron-vibration interaction in diradicaloids depends on the length of the π-electron conjugation when a paraphenylene group is inserted between the pyridine nuclei. It has been demonstrated that the evaluation of the strength of the electron-vibration interaction in cation-radicals is strongly dependent on the choice of a parameter for correction of the long-distance exchange interactions in TD-DFT methods, on the type of the compound and on the type of the excited state.

CONCLUSION

The presented materials fully meet in terms of volume and content the requirements of the Law for the Development of the Academic Staff in the Republic of Bulgaria, the requirements of Sofia University, and the requirements of FCP at Sofia University. The candidate is a scientist capable of solving complex scientific and applied scientific problems in the field of Theoretical Chemistry. I have personal impressions of Dr. Romanova from the course in Molecular Mechanics in the master's program in Computational Chemistry. I am very impressed by its scientific growth in the last 10-15 years - modern scientific issues and active international scientific contacts.

After getting acquainted with the materials presented by the candidate, scientific and scientific-applied contributions, and analysis of their significance, I confidently give my positive assessment and recommend the Scientific Jury to prepare a proposal to the Faculty Council of FCP-SU for election of Assist. Prof. Professor Dr. Julia Ruslanova Romanova in the academic position of "Associate Professor".

Prof. Petko Ivanov