STATEMENT

by Assoc. Prof. Dr. Miroslav Angelov Rangelov,
Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences
on the materials, submitted for participation in a competition for the academic position of Associate Professor in the professional field 4.2. Chemical sciences, scientific speciality 'Theoretical chemistry' for the needs of Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski" Announced in State Gazette No 21 of 15 March 2022.

In the competition for Associate Professor, announced in the State Gazette No. 21/15.03.2022 for the needs of the Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski" only one candidate participated, Dr. Iskra Zareva Koleva. For participation in the competition, the candidate has submitted a complete set of documents that satisfy and exceed the requirements of the Law for the Development of Academic Staff in the Republic of Bulgaria and the Regulations on the Conditions and Procedure for the Acquisition of Scientific Degrees and the Occupation of Academic Positions at Sofia University "St. Kl. Ohridski" and Faculty of Chemistry and Pharmacy. The candidate meets the criteria for the academic position of Associate Professor.

Iskra Koleva graduated in 2013 with a Bachelor's degree in Computer Chemistry and a Master's degree in Materials Science from the Faculty of Chemistry and Pharmacy, Sofia University, “St. Kliment Ohridski”. In 2017, under the supervision of Prof. Dr. Georgi Vayssilov and Assoc. Prof. Dr. Hristiyan Alexandrov, she successfully defended her PhD thesis "Quantum-chemical modelling of heterogeneous catalytic systems based on cerium dioxide" at the Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski". In 2017 she joined the Department of Pharmaceutical and Applied Organic Chemistry of the Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski" as a senior assistant professor. She has been holding this position for the present time.

Dr. Koleva is a co-author of 18 scientific publications in journals with impact factor, and she participated in the competition with 14 of them (11 publications - Q1 and 3 publications - Q2). Dr Koleva's habilitation thesis is based on four of the articles (all Q1), two of which Dr. Koleva is first

author. Dr. Koleva's Hirsch index is 7, the total number of citations, excluding self-citations, for all her publications is 208, and for the articles involved in the competition is 154.

Dr. Koleva has presented her scientific results at 22 national and international forums, where she has given 12 oral presentations and 10 poster presentations. She has also participated in the organization of one international and 9 national scientific conferences in the field of chemistry. She has been on 5 short-term research visits to Universitat de Barcelona, Spain.

Dr Koleva's scientific activity is also evident from the number of national (7) and international (3) research projects in which she has participated, four of them were used in the competition (indicator G).

The teaching and pedagogical activity of the candidate includes the teaching of practical classes in the Master's and Bachelor's courses: Hybrid (QM/MM) Methods, Modeling of Periodic Systems and Nanostructures, Computer Methods in Spectroscopy, Pharmaceutical Analysis Part I and II, Instrumental Methods in Chemistry Part II, Biopharmaceutics. Dr. Koleva has also been a thesis supervisor for one thesis of Master's student.

The scientific contributions of the included articles are in the field of theoretical quantum chemical research. In her habilitation thesis, Dr Koleva has presented four papers in which quantum chemical calculations have been used to theoretically study problems related to heterogeneous catalysis.

The main part of it is devoted to theoretical model investigations of parameters important for the catalytic properties of Zr^{+} and Y^{+} doped cerium dioxide surfaces and nanoparticles. The distribution of dopants in doped cerium dioxide systems, the influence of different amounts of dopants, and also their influence on the reducibility of CeO_2 are elucidated.

A separate quantum chemical study aims to shed light on the difficult to observe experimental changes in the electronic structure of platinum catalysts interacting with CO. The influence of CO on different size models of platinum clusters and nanowires deposited on CeO_2 is investigated. Theoretical thermodynamic and kinetic studies on the interaction of carbon atoms with various nanoparticles and crystal surfaces of noble and base metals are also presented. The thermodynamically stable positions of the carbon atoms, as well as the barriers associated with their displacement between the subsurface and surface layers of the metal, are established. Some of the catalysts investigated by Dr. Koleva have a high potential for implementation in practice due to their high activity and relatively lower cost compared to currently used noble metal-based catalysts.

The articles included in the competition for indicator D are also in the field of quantum chemistry and are focused both on the interactions between organic molecules and zeolites and mesoporous

silicates, as well as on the complexes of various trivalent metals with cucurbiturils with different ring sizes.

Conclusion

The overall scientific activity of the candidate is in the field of theoretical chemistry, which completely matches the professional field of the announced competition. The publications submitted by the candidate are on the topic of the competition and are original and innovative scientific research with a significant contribution to the theoretical heterogeneous catalysis. As a result of the foregoing analysis of the submitted materials I am convinced in my positive assessment for the candidate Dr. Iskra Koleva which fully meets all the requirements of the Law for holding the academic position of "Associate Professor" and I propose that she will be elected as "Associate Professor" in the professional field 4.2. Chemical sciences (Theoretical Chemistry) in Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski".

07.07.2022

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