

## Opinion

on the presented materials of Dr. Iskra Zareva Koleva for participation in the competition for associate professor of Theoretical Chemistry at the Department of Pharmaceutical and Applied Organic Chemistry, Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski", announced in SG no. 21/2022,  
by Prof. Dsci Boris Simeonov Galabov

Iskra Zareva Koleva obtained a higher education - a bachelor's degree in Computer Chemistry in 2012, and a year later a master's degree in Materials Science at the Faculty of Chemistry and Pharmacy. During the period 2014-2017 she was a full-time doctoral student in theoretical chemistry under the supervision of Prof. Georgi Vayssilov. She successfully defended a doctoral dissertation and since 2017 has been a senior assistant at the Department of Pharmaceutical and Applied Organic Chemistry, FHF. Her dissertation is on "Quantum chemical modeling of heterogeneous catalytic systems based on cerium dioxide." Senior assistant Iskra Koleva has so far published a total of 18 scientific papers, entirely in established international scientific journals. She participates in the competition with 14 scientific publications. 11 articles are in quartile Q1 journals, and the remaining 3 in quartile Q2 journals. These facts underline the solid scientific level of the candidate's work. These scientific publications have been cited 154 times in the specialized literature for the past few years. The candidate has participated with oral presentations or posters in 23 scientific conferences. She has also participated as a member of the working team in ten national and European research projects. During the period 2017 - 2022 she is engaged in teaching and supervision of practical and seminar classes for six courses in the fields of pharmaceutical analysis, biopharmacy, instrumental methods in chemistry and theoretical modeling in chemistry.

All indicators of the minimum requirements for obtaining the scientific title "Associate Professor" are met, and in most indicators the points are exceeded. All the data discussed above testify that the candidacy of Dr. Iskra Koleva fully complies with the state

requirements, as well as with the specific requirements of Sofia University for the fields of chemistry and pharmacy. The scientific contributions of the candidate are in the field of theoretical modeling of solid phase materials - zeolites, silicalites, catalytic systems containing cerium dioxide - their interaction and modification with metal cations and organic molecules. In addition, nanoparticles of transition metals were studied and characterized, as well as the host - guest interaction of metal ions with cucurbituric macrocycles. It should be emphasized that in most scientific papers the theoretical calculations of Iskra Koleva are closely related to experimental studies conducted by co-authors, aimed at characterizing the properties and interactions of catalytic systems important for technology. Reliable methods of density functional theory are used, combined with basic sets describing the studied systems and interactions with sufficient accuracy. Therefore, the obtained results and the conclusions made correlate very well with the available experimental data. The obtained theoretical predictions are solidly substantiated. Each of the publications is of independent scientific interest in the chemistry and physics of the studied complex systems. It is no coincidence that Iskra Koleva's publications are in leading international scientific journals in the field of chemistry.

The scientific contributions of Dr. Iskra Koleva are impressive. I will emphasize just a few.

- It has been shown by theoretical modeling that subsurface carbon particles are an integral part of nanoparticles on metal surfaces for Pd, Ni, Pt, Cu, Au and Ag. Carbon structures can form a partial positive charge, important for the catalytic properties of these metals (*Angew. Chem.* 2019).

- Periodic calculations have clarified the changes in the electronic structure and geometry of platinum clusters and nanowires induced by their deposition on the surface of oxides as well as the resulting adsorption of carbon monoxide (*Catal. Today*, 2019).
- The stability of cerium dioxide nanoparticles as a function of the amount of zirconium additives has been clarified by periodic DFT computations (*PCCP*, 2020).
- Theoretical calculations conducted by the candidate show the mechanism of formation and provide characterization of properties of superelectrophilic metal cations in Pd/ SSZ-13 zeolite. This result is a novelty in the literature. It has been convincingly shown that palladium ions in the zeolite are in the form of superelectrophilic Pd<sup>2+</sup> ions, previously identified in the literature as Pd<sup>3+</sup> and Pd<sup>4+</sup> ions. Various experiments have proved the theoretical results (*J. Phys. Chem. C*, 2020).
- One of the studies directly aimed at practical use is the investigation on the use of atomically dispersed palladium in zeolite SSZ-13. This material completely eliminates CO and NO<sub>x</sub> waste gases and is suitable for use in automotive catalysts (*Angew. Chem.* 2018).

Dr. Iskra Koleva is an excellent teacher and enjoys the respect of students. She pays special attention to her teaching work. She is expected to give lectures on Instrumental Methods in Chemistry from the next semester. In view of the above, I strongly support the award of the scientific title "Associate Professor" in theoretical chemistry to Dr. Iskra Zareva Koleva, a truly convincing candidacy.

June 24, 2022.

Reviewer:



/ Prof. DSci Boris Galabov /