OPINION

in a competition for selection of an "associate professor" in a professional field 4.2. "Chemical Sciences" (Theoretic Chemistry) for the needs of the Faculty of Chemistry and Pharmacy, Sofia University “St. Kliment Ohridski”, announced in State Newspaper no. 21/15. 03. 2022

Reviewer: Prof. DSc Tanya Stoyanova Tsoncheva (Hristova), Institute of Organic Chemistry with Center for Phytochemistry, Bulgarian Academy of Sciences

on the basis of the order No. РД-38-192/12. 04. 2022 г. of the Rector of Sofia University “St. Kliment Ohridski”

Candidate for the competition: Dr. Iskra Zareva Koleva, Assistant Professor in the Department of the Pharmaceutical and Applied Chemistry, Faculty of Chemistry and Pharmacy, Sofia University

Professional biography of the candidate

Iskra Koleva was born in 1989. In 2013 she graduated with a master's degree of "Materials Science" in the Faculty of Chemistry and Pharmacy, Sofia University. In 2017 she defended her doctoral dissertation in "Theoretical Chemistry" on "Quantum-chemical modeling of heterogeneous catalytic systems based on cerium oxide" at the same faculty. Since 2017, she has held the position of Assistant Professor in the Department of Pharmaceutical and Applied Chemistry, in Faculty of Chemistry and Pharmacy, Sofia University.

Teaching activity

In the last 5 years, Assistant Professor Dr. Iskra Koleva leads exercises in the bachelor's program "Instrumental Methods in Chemistry" and a number of master's programs, such as: "Pharmaceutical Analysis", "Computer Methods in Spectroscopy", "Hybrid (QM / MM) Methods", "Modeling of periodic systems and nanostructures ”and “ Biopharmacy ” with a total employment of over 1700 hours. She was the supervisor of 1 graduate student.

Research activity

The scientific activity of Dr. Iskra Koleva is mainly related to theoretical research in the field of heterogeneous catalysis. In this field, she has co-authored 18 scientific papers in impact factor journals. Of the 14 publications included in the competition, 11 were published in journals with quartile Q1 and 3 - with Q2). 154 citates were noticed on them. Some of the results are presented through oral or poster presentations at over 10 scientific forums. She actively participates in the organization of national and international conferences. Many times she is a member of the research

team of national and European projects. The h-factor, according to data from SCOPUS, is 6. She is the winner of the L'Oréal and UNESCO award "For Women in Science" in 2020.

Habilitation thesis

Dr. Koleva's habilitation thesis is dedicated to "Quantum chemical research of heterogeneous catalytic systems containing cerium dioxide and metal nanoparticles". It includes results published in 4 prestigious scientific journals, 3 of which are with quartile Q1 and 1 with quartile Q2. In two of the publications, the candidate takes the first place in the author's team, and in the others - the second place.

Cerium oxide particles of diverse size, doped with different amounts of Zr^{4+} ions, were modeled. For the system containing one Zr^{4+} ion, it was found that regardless of the size of the cerium oxide particle, the most stable substitution is in the subsurface position. It has been proven that for relatively large particles with a higher content of Zr^{4+} ions it is energetically more advantageous to replace the subsurface positions, as the stability of the system is commutative and is determined by the stability of occupied positions in 1 Zr^{4+} substitution models. Studies on the formation of oxygen vacations in these materials show the favorable importance of Zr^{4+} substitution, with vacations close to dopant being the most stable. The removal of four-coordinated oxygen centers has been shown to be most advantageous for larger nanoparticles.

Substitution of Ce^{4+} with an aliovalent ion (Y^{3+}) in CeO_2(111) surfaces is most energetically advantageous when Y^{3+} ions are located in the subsurface layer and there is a compensation oxygen vacation near them. For smaller CeO_2 particles, a preferred Y^{3+} position and oxygen vacation have not been established. For larger particles, a high stability of the structure was found, in which Y^{3+} cations are symmetrically located on the top of the particles and a vacation was formed by removing a two-coordinated O center from (100) facets. The optimization of the ions location during the development of a second vacancy is discussed. For particles with a higher yttrium content, it has been proven that the formation of O-vacancies at diagonally opposite positions or at two opposite (100) facets is the most energetically advantageous.

Theoretical calculations on the adsorption of CO on platinum clusters deposited on CeO_2 are of great practical importance. Models have been optimized, including different orientations of the adsorbed molecule, varying the degree of surface coverage with CO, and changes in the size of the platinum cluster. The effect of the nature of the carrier was studied by comparison with similar samples supported at Al_2O_3. It has been shown that, in contrast to smaller platinum clusters, the adsorption of CO on platinum wires is preferred bridging. Theoretical calculations show that the difference in density of 5d Pt levels is insignificant for relatively smaller clusters when they are deposited on CeO_2

and changes with the use of Al_2O_3 as a support, as a result of electron transfer from Pt particle to the support. It is concluded that the reactivity of platinum particles decreases with increasing their size and with increasing degree of surface coverage with CO.

Studies on the interaction of carbon with metals (Cu, Ag and Au) are related to the deactivation and, in some cases, to the promotion of catalysts. Both metal nanoparticles and surfaces are modeled. Low-coordinated metal centers have been shown to favor sub-surface positions of C, which is particularly pronounced for Cu and Ag, but this effect decreases at higher degrees of coverage. Stabilization of the internal electronic levels of metal atoms as a result of their interaction with C is shown, which implies the occurrence of a partial positive charge. The conclusion made on the basis of the phase diagrams regarding the increased thermodynamic stability of isolated C atoms on Cu, Ag and Au surfaces under the conditions of catalytic reaction is very important.

Scientific contributions of research not included in the habilitation thesis

The results of the research outside the habilitation work were published in 8 publications with quartile Q1 and 2 with Q2. They are dedicated to quantum chemical modeling of zeolites containing metal cations and the interaction of molecules with metal ions and surfaces.

I believe that the main contributions of the research are related to the assessment of the complexation of cucurbiturils with Al^{3+}, Ga^{3+}, In^{3+}, La^{3+} and Lu^{3+} ions in gas phase and aqueous medium, taking into account the effect of macrocycle cavity size and pH; elucidation of the influence of the nature of surface functional groups on mesoporous silicas on the adsorption of miltefosine, tamoxifen and curcumin; study of the influence of Si defects or substituted in the zeolite lattice heteroatoms (Al^{3+}, Ti^{4+}) on the adsorption of hydrogen peroxide, pyridine and acetonitrile; modeling the formation of carbonyl, nitrosyl or mixed carbonyl-nitrosyl complexes in Pt- or Pd-modified zeolites; research on the effect of paraquat on ion exchange in zeolites; comparison of the stability of iron ions at different positions in zeolites.

Conclusion

The documents submitted for review by Dr. Iskra Koleva show that she is a very good researcher and an approved specialist in the field of quantum chemical modeling of materials. The candidate's theoretical research on a variety of systems, including the interaction of metal / metal ions and various molecules with surfaces and nanoparticles, is important to clarify and optimize the properties of materials for application as adsorbents and catalysts. The active publishing activity of the candidate, the wide citations of the results in foreign literature, combined with her leading activity in much of the research, and last but not least, the active teaching activity, do not doubt that Dr. Koleva fully meets the requirements of the current competition. Therefore, I strongly recommend to the esteemed

Faculty Council of the Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski" to award Dr. Iskra Koleva the academic position of "Associate Professor" in the professional field 4.2. "Chemical Sciences", scientific specialty "Theoretical Chemistry".

6.06.2022 Prepared the opinion:

Sofia /prof. DSc.Tanya Tsoncheva/