REVIEW

by Assoc. Prof. Dr. Galia Kostova Madjarova

Chair of the scientific jury on an open procedure for the academic position "Associate Professor" in Professional field 4.2. Chemical sciences (Theoretical Chemistry) for the needs of department of Pharmaceutical and Applied Organic Chemistry, Faculty of Chemistry and Pharmacy at Sofia University "St. Kliment Ohridski", announced in State Gazette 21/15.03.2022.

The only applicant for the position is Chief Assistant Prof. Dr. Iskra Zareva Koleva. The candidate has submitted all documents and materials required by law.

Dr. Iskra Koleva is a graduate of the FCP at SU "St. Kl. Ohridski". In 2012, she graduated as a BSc in Computer Chemistry with excellent grades, and in 2014 obtained MSc in master's program "Materials Science". From 2014 to 2017, she was a doctoral student at the Department of Organic Chemistry and Pharmacognosy at SU, with scientific supervisors Prof. G. Vayssilov and Prof. Hr. Alexandrov. In 2017, she successfully defended PhD thesis on "Quantum-chemical modeling of heterogeneous catalytic systems based on cerium dioxide". Since 2017, she works as Ch. Assistant Professor in the Department of Pharmaceutical and Applied Organic Chemistry. From 2018 to 2020, she has accomplished five short-term visits at the University of Barcelona in Spain, where she has established a successful collaboration, evident from the publications. For the achieved scientific results, in 2020, Dr. Iskra Koleva won the award "For women in science" – a program of L'Oréal and UNESCO.

Dr. I. Koleva is a co-author of **18** scientific publications, two of which are included in the PhD thesis for obtaining educational and scientific degree "Doctor". She participated in the current selection procedure with **14** publications (11 publications – Q1 and 3 publications – Q2), and the habilitation thesis is based on **4** of them. The noticed citations of the publications submitted for evaluation **154**, and the total number of citations to all publications is **168**. All articles submitted for participation in the current procedure were published in international journals with an impact factor, and **2 of them** were in journals with an impact factor **greater than 15.0**. The Hirsch index of Dr. I. Koleva at the time of submitting the documents is **h=6**. Currently, she participates in **3** national and **1** international project. Dr I. Koleva has presented her scientific results at **14** national and international conferences and workshops. She also has personal experience in organizing scientific conferences such as: FEZA 2017 - Conference of the Federation of European Zeolite

Associations; National Chemistry Conference for Undergraduates and PhD Students in the period 2013-2022.

Scientific Research activities

The scientific research activity of Dr. I. Koleva is focused in the field of quantum chemical modeling of systems used in heterogeneous catalysis and drug delivery systems based on mesoporous silicates.

Dr. I. Koleva presents a habilitation thesis "Quantum-chemical study of heterogeneous catalytic systems containing cerium dioxide and metal nanoparticles" were in 37 pages the results of articles [4,6,10 and 13] are summarized. Part of the research naturally extends scientific investigations in the study subject of the PhD thesis. The change in the catalytic properties of CeO_2 upon its doping with zirconium and yttrium is systematically studied [4,13]. Different nanoparticle models are examined to establish the effect of particle size and models with different positions of the dopant ions. CeO_2 model systems are improved by deposition of Pt clusters and nanowires on which CO molecules are adsorbed [6]. For comparison, models of Al_2O_3 with platinum nanoparticles deposited on it were calculated. Publication [10] is devoted to the role of carbon in heterogeneous catalytic processes. The thesis describes the essence of the research carried out and highlights the original results that have been achieved.

The publications, outside of the habilitation thesis, can be divided into several directions.

• Quantum-chemical modeling of zeolites containing metal cations [2,7,8,9,12,14]

The presence of metal ions in various zeolite structures greatly affects their catalytic activity. Using density functional theory, the explanation of the experimental structural data and mechanisms of the processes are proposed.

Publications [7, 12] are focused on zeolites with small pores of the chabazite type with atomically dispersed Pt and Pd, which have a potential application for passive adsorption of nitrogen oxides and CO. These model systems were used to investigate and understand the influence of transition metals in microporous materials. It is shown that the studied material can be used for the simultaneous removal of CO and NOx, and the mechanism of action is clarified. Research on this topic had found a wide response in the scientific community.

Theoretical study of Ti-MCM-68 zeolite [2], which can activate hydrogen peroxide clarify the stability of structures with different positions of Ti, combined with the presence of defects (silanol nests). By evaluating the relative stability of the silanol nests and the substitution of Si

with Ti or Al in different crystallographic positions, the catalytic activity of the investigated zeolite system is described. The adsorption of small organic molecules in the zeolite is also modeled and the influence of silicon vacancies on the catalytic activity is evaluated.

Combined experimental and theoretical studies in publication [8] evaluate the interaction of the herbicide paraquant with NaY zeolite samples with different Si/Al ratios and pore sizes. The modeling shows the preferred arrangement of the paraquantum molecules in the zeolite structure, which helps to understand the observed results for the absorption behavior of the studied zeolite systems.

Different iron-containing HZSM-5 zeolites were modeled [9] and the relative resistance of different Fe-containing cations in the zeolite pores is elucidated. The obtained conclusions are supported by the experimental results and explain the observed temperature evolution.

The ability of cation-exchanged zeolites containing extra-framework alkali and alkaline earth metal ions (Li^+, Na^+, K^+ and Ca^{2+}) to improve the stability of palm oil against heat treatment and oxidation is analyzed [14]. Quantum chemical calculations of the model systems explain the experimental observations and show that the metal ions preferentially trap the peroxide, which slows down the oxidation of palm oil.

• Quantum-chemical modeling of drug delivery systems based on modified mesoporous silicalites [3,5 and 11]

Publication [5] is a combined study of a drug-delivery system based on magnetic silicate nanoparticles, which has the ability of targeted drug delivery in the body. The characterization of the obtained nanoparticles and their interaction with tamoxifen are promising results. Theoretical modeling shows that hydrogen bonds between the drug and the modified surfaces are key factor to the stability of the adsorption complexes. Magnetic silicon mesoporous systems smaller in size and obtained by different methods were characterized in pulication [3] and their interaction with miltefosine is investigated. The mechanism of drug molecule adsorption has been clarified.

Publication [11] characterized the interaction of curcumin with mesoporous silicate nanoparticles further functionalized with amino groups. The nanoparticle has been investigated as a potential drug delivery system. The research is complex and combines multiple experimental methods of analysis and theoretical modeling. The structure of the most stable complexes is proposed and the mode of coordination of curcumin is clarified at the molecular level.

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• Quantum-chemical modeling of the interaction of trivalent metal cations with cucurbiturils [1].

The theoretical study clarifies the mechanism of formation of complexes between the trivalent ions (Al^{3+}, Ga^{3+} In^{3+} La^{3+} and Lu^{3+}) and cucurbiturils. The structure and thermodynamic stability of the model systems are discussed and the key factors for increasing the water solubility of the macrocyclic system are outlined.

The scientific publications presented for evaluation correspond to the professional field of the opened academic position and are in the area of theoretical computational chemistry. A significant part of the scientific publications of Dr. Iskra Koleva are done in collaboration with experimental groups. Presented research enriches scientific knowledge by clarifying the structure of the studied systems and offering materials with improved properties or new functionalities.

Teaching activities

Dr. Koleva teaches in bachelor's and master's programs of the FCP.

BSc level – practicum in “Instrumental methods in chemistry”- Part II (major Chemical Engineering and Contemporary Materials)

MSc level - practicum in “Hybrid QM/MM Methods”, “Modelling of periodic systems and nanostructures” and “Computational Methods in Spectroscopy" for the M. Sc. program “Computational Chemistry” and practicum in "Pharmaceutical Analysis" Part I and II and "Biopharmacy" for major "Pharmacy".

Dr. I. Koleva was the supervisor of one master's thesis.

The regular teaching activity of Dr. Koleva shows a serious commitment to the educational process in the department and the faculty. The work with the students also finds positive feedback in the surveys that the students fill out at the end of each semester.

Dr. Iskra Koleva is a reliable colleague and my personal impression of her is excellent.

Conclusion

The candidate Dr. Iskra Koleva is an active researcher in the field of theoretical chemistry with a scientific output entirely focused on the professional field of the opened position.

The presented materials fully comply with all the requirements of the Regulations for the terms and conditions for acquiring scientific degrees and holding academic positions at SU "St. Kliment Ohridski", as well as the additional, recommended specific criteria for professional field 4.2 "Chemical Sciences" of the Faculty of Chemistry and Pharmacy. Based on the above, I consider that Ch. Assist. Prof. Dr. Iskra Zareva Koleva fully satisfies the conditions for the appointment of the academic position of "Associate Professor".

I confidently give my positive assessment and recommend to the Faculty Council of the Faculty of Chemistry and Pharmacy at Sofia University "St. Kliment Ohridski" to vote Dr. Iskra Zareva Koleva to be appointed for academic position of "Associate Professor" in professional field 4.2 Chemical Sciences (Theoretical Chemistry).

Sofia, July 11, 2022 Reviewer: Galia Madjarova Digitally signed by Galia Madjarova Date: 2022.07.11 09:20:51 +03'00'

(Assoc. Prof. Galia Madjarova)