R E V I E W

on the application for **Professor position**
in Chemical sciences (Organic Chemistry – Organic Catalysis)
announced in the Bulgarian State Newspaper, vol. 52 from July 02, 2019

by Prof. Dr. **Anela Nikolova Ivanova**, Sofia University, Faculty of Chemistry and Pharmacy, Chair of the scientific jury appointed with Order № 38-445/16.07.2019 of the Rector of Sofia University

There is a single applicant for the position – Assoc. Prof. Dr. Hristiyan Aleksandrov Aleksandrov. All required documents are available, together with information on additional criteria related to the selection procedure.

The applicant has graduated Sofia University as a B. Sc. in Chemistry with excellent grades in 2002. Since 2008 he holds PhD in Organic chemistry after successful defense of his PhD thesis „Theoretical study of the structure of zinc-containing ions in the pores of ZSM-5 zeolites and the mechanism of ethane dehydrogenation therein". Dr. Aleksandrov has worked as a Senior Assistant Professor from 2009 till 2014 at the Department of Organic Chemistry, Faculty of Chemistry, Sofia University "St. Kliment Ohridski". In the last 5 years and 4 months he has been Associate Professor in Organic Chemistry at the Department of Organic Chemistry and Pharmacognosy of the Faculty of Chemistry and Pharmacy (FCP) of Sofia University.

Dr. Aleksandrov has teaching experience with lectures and lab courses in Organic Chemistry 1 for several B. Sc. majors and with lectures in "Modelling of periodic systems and nanostructures" for the M. Sc. programme "Computational Chemistry". The students in the latter are very positively impressed by him as a teacher. The average teaching load of the candidate for the past 4 years is 372 academic hours.

Dr. Aleksandrov is a co-author of: 58 scientific publications, 57 of which published in international journals with impact factor, of 2 book chapters, and of 1 didactic aid. He has submitted for the selection procedure 36 publications (all of them in international peer-reviewed journals) and 1 didactic aid. None of these has been used for the position of Associate Professor or for the PhD degree. Hence, in line with Art. 29, Sec. 1, P. 3, 4 of the Law for promotions in academia in Bulgaria (LPAB), they are used to evaluate the scientific contributions of the candidate. Dr. Aleksandrov is first author in 6 of the publications. Most of the latter are in very renowned and widely acknowledged specialized journals: Nature Materials (1 paper), Angewandte Chemie International Edition (3 papers), Chemical Communications (1 paper), Journal of Physical Chemistry C (7 papers), Physical Chemistry Chemical Physics (5 papers), ACS Catalysis (2 papers), Microporous and Mesoporous

Materials (3 papers). The publications submitted for assessment have been cited 209 times in international peer-reviewed journals. The total number of independent citations of the publications of Dr. Aleksandrov is 593 (Source: Scopus). The applicant has coordinated 1 national research project and participated in 22 national and 8 international projects. He has co-supervised 1 successfully defended PhD thesis. Dr. Aleksandrov has reported his results at 19 scientific events abroad and at 16 international and 7 national conferences in Bulgaria. He has been member of the organizing committee of 11 scientific fora. Dr. Aleksandrov is the recipient of 3 prestigious awards – 1 international (by Foundation „Bernd-Artin Wessels“), 1 national („Pythagoras“) and 1 university (Annual award of the Rector of Sofia University for 2002). The fact that he is an acknowledged specialist is corroborated by the fact that he was invited as a member of 5 scientific juries for appointments of Senior Assistant Professors and Associate Professors and that he is a reviewer of manuscripts submitted for publication in international scientific journals.

Dr. Aleksandrov presents the following achievements to fulfill the minimum national requirements for occupying the Professor position:

- indicators group A – defended PhD thesis - 50 points out of minimum required 50;

- indicators group C – habilitation thesis on the effect of adsorbed hydrogen on various catalytic materials, based on 6 publications in Q1 - 150 points out of minimum required 100;

- indicators group D - 30 publications not included in the habilitation thesis, 26 in Q1, 4 in Q2 - 730 points out of minimum required 200;

- indicators group E - 209 citations of the publications submitted for evaluation - 418 points out of minimum required 100;

- indicators group F – co-supervision of 1 PhD student, coordination of 1 national project (with secured third-party funding) and participation in 21 national and 8 international projects, co-author of 1 didactic aid – 427 points out of minimum required 150.

It is evident from the above summary that the applicant either fulfills or goes beyond the minimum national requirements in all groups of indicators. The overall scientific metrics is in compliance with the general requirements of LPAB, the statutes for its application, and the additional recommendations of FCP.

Dr. Aleksandrov has submitted for assessment also a habilitation thesis „Elucidation of the factors affecting the hydrogenation of alkenes on transition metals – a theoretical study“, where on 63 pages he has summarized the data obtained on this topic and published in 6 of the papers. The thesis is clearly written and concise and highlights the most important achievements of the applicant. Stepping up of the computations is evident.

The research of Dr. Aleksandrov is mainly in three directions: 1) theoretical description of the properties of species adsorbed on the surface of zeolites and nanoparticles

and their various applications in catalysis (27 papers); 2) computational characterization of the structure of solid materials (5 papers); 3) modelling of the application of zeolites as containers for drug transport (4 papers). The computational methodology is exclusively Density Functional Theory with specific implementation for solid state calculations. The added value of the obtained results is for clarifying the structure of materials at the molecular level and for providing additional information, which aids the understanding of the mechanisms of a number of catalytic reactions.

The computational studies in the first direction (№ 1, 3, 4-13, 15-23, 27, 28, 30-33) focus on determining the preferable positions for adsorption of different species (W, C, NO, CO) on surfaces. The models consist most often of metal clusters or zeolite fractions where one or several (groups of) atoms are adsorbed at different positions. As a result, it is demonstrated which are the most stable W-centres in an MFI zeolite and the effect of W on the structure and acidity of the zeolite is quantified. The selectivity of this system for CO_2 and NO_2 is explained. Stable complexes of Rh^+ and Pd^{n+} in faujasite zeolites are identified and a way to influence their catalytic activity, based on replacement of CO by NO, is suggested. The understanding of the mechanism of hydrogenation of ethene in dealuminated HY zeolites is supported. A stability series of Fe-containing ions in ZSM zeolites is put forward and after that confirmed experimentally. Special attention is paid to revealing the catalytic activity of CeO_2 at the molecular level. The type of sequentially forming N-containing adsorbates on its surface is elucidated, which supplements the information on the mechanism of catalytic conversion of NO. The influence of the adsorption of various number and type of Pt-ions/species on CeO_2 is traced in the absence and in the presence of CO. It is concluded that solely the vibrational bands of the oxide cannot be used to identify the type of adsorbed metal ions. Quantitative characterization is performed of the effect of CO concentration and of the presence of γ-Al_2O_3 or Y_2O_3 on the performance of CeO_2-based catalytic systems. It is shown that a MgO support affects weakly the adsorption of hydrogen on Pt and Pd nanoparticles and H-adsorption activation similar to that on Pd is discovered on Pt as well. New details are provided about the second stage of hydrogenation of ethene on Pd. The adsorption of C and O on Ni nanoparticles is investigated and critical maximum size of the particles for minimization of carbon deposits is suggested. The dissociation of O_2 on Pt nanoparticles is modelled and positive effect of surface flexibility and of inclusion of noble metals in the nanoparticle core is demonstrated.

The accent in the second research direction (publications № 25, 26, 34-36) is on the determination of the most preferable structures of standalone or complex-forming solid materials. This includes adsorption of paraquat in faujasite zeolites and of hydroperoxides and alkenes in M-X zeolites. Stable geometries and density of states of complexes of graphene with non-planar organic compounds are obtained.

The publications in the third research direction (№ 2, 14, 24, 29) aim to elucidate by quantum chemical calculations the interactions between drugs and their carrier. Mesalazine, quercetin, curcumin, and verapamil are the modelled drugs, while parts of zeolites are the carriers. It is explained why mesalazine does not stay in the zeolite and how quercetin binds to the surface of a pristine, NH_2- or Zn-modified silicalite, and curcumin – to that of a NH_2-functionalized silicalite. The influence of SO_3H and COOH groups on the coupling between verapamil and a silicalite is checked.

All studies are detailed and are conducted with proper quantum chemical methods after careful tuning of the computational procedure. In most of them, a theoretical explanation of experimentally observed phenomena is offered. The investigations are done in collaboration with experimental groups. The effect of various factors, which could influence the results, is verified without changing the complexity of the models. The latter contain the most essential components of the studied systems, which enable the derivation of qualitative and quantitative trends. All this outlines the high significance of the obtained results, which add new knowledge to the respective field.

The didactic aid is timely and useful because it contains instructions for lab experiments and a collection of Organic chemistry problems for solving by the Pharmacy students.

I would like to make the following recommendation to the work of the applicant at the new Professor position:

- to establish and endorse an independent research area in Organic catalysis, where he would have the leading role, which I am convinced that he is well prepared for.

It is worth noting that Dr. Aleksandrov is an excellent scientist and a valuable colleague. He works successfully both at the Department of Organic Chemistry and Pharmacognosy and at FCP. He initiates and maintains long-lasting collaborations with researchers from other institutions in Bulgaria and abroad. This delineates him as a prospective member of the academic community of FCP.

In summary, the materials submitted for the evaluation comply with all requirements of the law and with the additional recommendations of the Faculty of Chemistry and Pharmacy of Sofia University for a Professor position. This motivates me to assess positively the applicant Associate Professor Dr. Hristiyan Aleksandor and to vote for his appointment as a Professor.

October 28, 2019 Chair of the scientific jury:

/Prof. Dr. Anela Ivanova/