Attitude of Reviewer

Assoc. Prof. Dr. Momtchil Dimitrov Dimitrov, Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Ssciences

With respect to the competition for occupying the academic position "Professor" at Sofia University „St Kliment Ohridski", Faculty of Chemistry and Pharmacy (FCF), professional field 4.2. Chemical Sciences, scientific specialty "Organic Chemistry – Organic Catalysis", published in „Newspaper of State", issue 52/02.07.2019.

On the basis of Order № РД 38-445 dated 24.07.2019 by the Rector of Sofia University „St Kliment Ohridski", I have been appointed as member of the Scientific Jury in the competition for occupying the academic position 'Professor' in professional field 4.2. Chemical Sciences**,** scientific specialty „Organic Chemistry – Organic Catalysis", announced for the needs of Sofia University „St Kliment Ohridski", Faculty of Chemistry and Pharmacy". Assoc. Prof. Dr. **Hristiyan Aleksandrov Aleksandrov** from Sofia University „St Kliment Ohridski", Faculty of Chemistry and Pharmacy is the only candidate who submitted his application documents for participation in the announced competition.

The complete set of materials on a CD, submitted to me by Dr. Aleksandrov, is in accordance with the Law for the Development of the Academic Staff in the Republic of Bulgaria (LDASRB) and it comprises all required documents. The candidate participates in the competition with 36 scientific papers published in reputable international journals with impact factor (32 of Q1 rank and 4 of Q2 rank according to SJR) and with 1 scientific handbook for laboratory work in organic chemistry, which have not been included in his PhD thesis and have been published after occupying the academic position „Associate Professor". The total number of citations noted so far on them is 234. The total number of papers co-authored by the candidate is 61 (57 of which are published in journals with impact factor, 51 of Q1 rank and 6 of Q2 rank according to SJR), and the total number of citations noted so far on them is 637. The scientific results are presented personally by Dr. Aleksandrov at 55 national and international forums, 35 of them were oral (11 invited) and 20 poster reports. The submitted information on the minimum requirements for the applicant's scientific activity shows that for each of the indicators, Dr. Aleksandrov has the necessary number of points, and for most of them this number significantly exceeds the minimum national requirements.

The examination of the submitted materials shows that the applicant has a well-defined topic of interest and his scientific activity is in the field of theoretical modeling of the structure and properties of catalysts used in heterogeneous organic catalysis, and of the reactions that proceed on/within them. The author's reference is well prepared and in details competently reflects the scientific contributions of the applicant. The performed theoretical studies can be consolidated as follows: (1) Quantum-chemical modeling of zeolite systems containing cations and their complexes with applications in catalysis [scientific papers 26,34,40,42,49,50,54,55]; (2) Quantum-chemical modeling of catalytic systems based on CeO2 [scientific papers 30,31,33,35,37,38,39,44,45,48,52]; (3) Quantum-chemical modeling of transition metal nanoparticles and catalytic transformations on them [scientific papers 23,25,27,28,29,41,43,53]; (4) Quantum-chemical modeling of the interaction of organic molecules with zeolites and graphene [scientific papers 24,32,36,46,47,51,56,57,58]. I will not describe in detail all scientific contributions of the applicant, which are summarized well in the attached reference. I will emphasize only some of them. A successful approach for increasing the stability of MFI-type nanoscale zeolites by adding a tungsten source to the reaction mixture during synthesis is presented. Quantum-chemical calculations show that

W^{VI}=O are the most stable W-containing sites incorporated within the pores of this type of zeolite. The presence of W has been shown to prevent the formation of silanol groups by forming flexible W–O–Si bridges that are more stable than Si–O–Si bonds in pure silica zeolites. In another study, quantum-chemical calculations showed that the heterolytic dissociation of H_2 was highly endothermic on Al/O or Si/O sites in the zeolite structure but exothermic on extra-framework Al-containing particles, indicating that the combination of Broensted acid sites with extra-framework Al-containing particles is essential for the hydrogenation processes when no transition metal cations are present in the zeolite.

The comparison of the results obtained from periodic quantum-chemical calculations with the experimental results on catalytic systems based on CeO_2 [scientific papers 30, 31, 45] shows that the interaction of NO with reduced cerium dioxide leads to the formation of azides (N^{3-}) and nitrogen oxide anion (NO^{2-}), which is accompanied by oxidation of Ce^{3+}, and the formation of these surface compounds has been detected for the first time by the adsorption of NO on solid surfaces. In another study, the use of periodic quantum-chemical calculations based on density functional theory investigated the local structure and preferred positions for yttrium cations and oxygen vacancies in Y-doped ceria. It is shown that the doping does not significantly alter the reducibility of ceria systems, but it selectively facilitates the formation of oxygen vacations on the surface of doped ceria compared to pure ceria.

In a series of scientific papers [24,36,46,51,58], the interaction between different drugs and mesoporous silicate carrier in controlled drug delivery systems has been studied in detail via molecular quantum modeling. In papers 47 and 56, the structure and density of states of graphene were modeled, and complexes of graphene with non-planar organic compounds such as triphenylmethyl radical, anion and cation were investigated. The results obtained show that the geometry of the organic molecules does not change significantly, but the changes in the density of the electronic states of graphene make possible the identification of the complex formed.

In the applicant's Habilitation work (63 pages), the factors affecting the hydrogenation of alkenes on transition metals are studied in great detail.

Conclusion

The scientific achievements of Associate Professor Dr. Aleksandrov are undoubted and fully correspond to the topic of the announced competition. The submitted academic papers after habilitation, the number of citations, the participation in projects and the project management by the applicant not only meet, but also significantly exceed the requirements for occupying the academic position "Professor" according to LDASRB and the Regulations for the implementation of LDASRB.

On the basis of the above considerations, I strongly propose to the honorable members of the scientific jury to bestow to Associate Professor Dr. **Hristiyan Aleksandrov Aleksandrov** the academic position **"Professor"** at Sofia University „St Kliment Ohridski", Faculty of Chemistry and Pharmacy"**,** in the professional field 4.2. Chemical Sciences, scientific specialty "Organic Chemistry – Organic Catalysis".

Sofia, 26.10.2019 Member of the Scientific Jury at Sofia University", FCF:

(Assoc. Prof. Dr. Momtchil Dimitrov)