

REPORT

on the materials presented for participation in the competition, published in „*State Gazette*”, issue 52/02.07.2019 for occupying the academic post “Professor” in professional field 4.2 “Chemical Sciences”, scientific research specialty “Organic Chemistry – Organic Catalysis” for the needs of Faculty of Chemistry and Pharmacy at Sofia University “St. Kliment Ohridski”

Candidate: **Associate Professor Dr. Hristian Aleksandrov Aleksandrov**

Reviewer: Prof. Yuri Kalvachev, Institute of Catalysis, Bulgarian Academy of Sciences

The only candidate in the competition is Assoc. Prof. Dr Hristian Aleksandrov, who works in the same Faculty.

Hristian Aleksandrov graduated from the Faculty of Chemistry at Sofia University “St. Kliment Ohridski ”(present Faculty of Chemistry and Pharmacy) in 2004 as a Master of Chemistry. The following year he enrolled as a PhD student in the same Faculty after winning a competition and successfully defended educational and scientific PhD degree in 2007 and enrolled as an assistant in the Department of Organic Chemistry at the Faculty of Chemistry, Sofia. In 2014 he was appointed associate professor in the same department. He has specialized for 13 months as a postdoctoral fellow at the Faculty of Chemistry of the Technical University, Munich and 18 months at the Faculty of Chemistry of the University of Barcelona. In 2014, he received the prestigious Pythagoras Award for Young Scientist.

The research activity of Assoc. Prof. Dr. Hristian Aleksandrov is in the field of theoretical modeling of the structure of catalysts used in heterogeneous organic catalysis and theoretical modeling of chemical reactions occurring on catalysts. Very interesting are works investigating the interaction of organic molecules with zeolites and graphene by studying the properties of supports for controlled drug delivery, for neutralizing herbicides or for enhancing the stability of palm oil. Of great value in these studies is the combination of quantum-chemical calculations with experimental results.

The candidate, Hristian Aleksandrov, present in the competition 36 publications, all in Impact Factor journals. It is impressive that 32 of them are in the journals Q1 (first quartile, by WoS and Scopus categorization) and 4 are Q2 (second quartile), ie. the articles have been published in the most renowned international journals in the respective field - The Journal of Physical Chemistry; Physical Chemistry Chemical Physics; Applied Catalysis B: Environmental; Microporous and Mesoporous Materials. These works have found a wide response in the

scientific literature - they have 234 citations. The Hirsch index (h-index) of Assoc. Prof. Hristian Aleksandrov, verified in the Scopus scientific information database without self-citations, is 14, which indicates the high quality of work and the up-to-date tasks. The works submitted are original and relevant to the subject of the announced competition.

Information provided on the research work of Assoc. Prof. Dr. Hristian Aleksandrov is complete and fully represents the applicant's contributions.

The applicant's contributions can be summarized in the following areas:

(1) Quantum-chemical modeling of zeolite systems containing cations and their complexes with applications in catalysis;

(2) Quantum-chemical modeling of catalytic systems based on CeO₂. Various catalytic systems have been investigated in which metals or metal oxides are deposited on cerium oxide.

(3) Quantum-chemical modeling of transition metal nanoparticles and catalytic transformations on them. Important catalytic processes have been investigated such as: reforming of methane with CO₂, hydrogenation of ethene, dissociation of an oxygen molecule, influence of carbon on deactivation of catalytic systems

(4) Quantum-chemical modeling of the interaction of organic molecules with zeolites and graphene. The interaction of drugs, herbicides and other organic molecules with porous materials has been investigated.

The candidate Hristian Aleksandrov meets the requirements for occupying the academic post "professor" in Faculty of Chemistry and Pharmacy – Sofia University, referred to in Article 29, Paragraph 1, Items 3,4 and 5 of the Law on the Development of the Academic Staff in the Republic of Bulgaria and in the Regulations for its implementation, as well as the enhanced criteria of the Faculty.

All other requirements of the above mentioned law are fulfilled - a recognized educational and scientific degree "Doctor" and an academic position "Associate Professor". Diplomas are presented, as well as a certificate of employment showing that he had held the academic position of associate professor for a period longer than the required by the same law. A careful review of the materials submitted to me for review gives me a reason to claim that there is no evidence of plagiarism in the scientific works of Assoc. Prof. Hristian Aleksandrov and he fulfills the condition referred to in Article 29, Paragraph 1, Item 6 of the law. Additional basis for this is the publication of papers in reputable journals that monitor plagiarism.

The habilitation work of Assoc. Prof. Aleksandrov has been prepared at a high scientific level and is entitled "Clarification of the factors affecting the hydrogenation of alkenes on transition metals - a theoretical study". The work is based on 6 articles, all published in the journals of the first quartile Q1. The contribution of these works is to clarify the reaction mechanisms of this reaction to various catalytic systems and to study the factors that influence them. These

contributions open the door to modeling more complex systems based on quantum-chemical methods and applying them to new research problems.

Assoc. Prof. Hristian Aleksandrov meets and exceeds the requirements of Art. 29, para 1 of the Law on the Development of the Academic Staff in the Republic of Bulgaria and in the Regulations for its implementation, as well as the enhanced criteria of the Faculty of Chemistry and Pharmacy – Sofia University.

The above gives me a reason to assess positively the candidature of Dr. Aleksandrov and to recommend to the Scientific Jury to prepare a report-proposal to the Scientific Council of Faculty of Chemistry and Pharmacy for the election of Associate Professor Dr. Hristian Aleksandrov Aleksandrov as a Professor in the professional field 4.2. “Chemical Sciences”, scientific research specialty “Organic Chemistry – Organic Catalysis” for the needs of Faculty of Chemistry and Pharmacy at Sofia University “St. Kliment Ohridski”.

October 25th, 2019

Sofia

Prof. Yuri Kalvachev