**COMENIUS UNIVERSITY IN BRATISLAVA**
**FACULTY OF NATURAL SCIENCES**
**DEPARTMENT OF PHYSICAL AND THEORETICAL CHEMISTRY**
Ilkovičova 6, 842 15 Bratislava 4, Slovakia

Date: 2019-23-07

**Report on habilitation thesis of Mgr. Piotr Błoński, Ph.D.**

I am pleased to provide my assessment of the habilitation thesis of Dr. Błoński (hereafter referred to as "author") entitled "Atomic clusters and graphene: many faces of nanomagnetism". The submitted thesis consists of four chapters providing a brief introduction to the magnetism, overview of the methodology used throughout the work discussed in the thesis, presentation of the main results, and summary and outlook recapping the most important achievements. The chapter "Results" is based on the material from 17 research articles published in leading peer-reviewed journals that are provided as appendices 1-3. It is worthwhile to mention that Dr. Błoński is listed as the first author in most of the listed papers (12 out of 17).

A major part of the Results chapter (sections 3.1-3.4) presents a series of works motivated by the search for a magnetic storage medium with a large data storage density. In these studies, small homo- and hetero- nuclear transition metal clusters acting as molecular magnets were chosen as the objects of interest and their main property explored was the magnetic anisotropy energy (MAE) determining the barrier of magnetization reversal due to thermal excitations. I particularly appreciate the author's systematic and purposeful approach to his research subject. At the first stage, structure and magnetic properties of free-standing homo- and hetero- nuclear clusters (ranging from dimers to hexamers) have been explored. The physical mechanism determining the variation of MAE and the influence of spin-orbit coupling on the structural and magnetic properties of clusters have been studied in detail. Nevertheless, the use of the free-standing clusters would be highly impractical in real applications. The logical next step therefore was to consider the clusters deposited on a substrate. As demonstrated in section 3.2, even the use of a relatively weakly interacting substrate graphene leads to a substantial modification of the magnetic properties of monometallic Pt and bimetallic Pt-Co, Pt-Fe, and Ir-Co clusters. Next, the structural model was extended to contain metallic substrates providing support for the graphene sheet. In this context, Pt clusters on graphene supported on Ni(111) and Cu(111) surfaces is discussed. In all these studies, a very detailed and insightful analysis of the electronic structure, magnetic properties, and geometry is provided and the observed trends are carefully explained and interpreted. All the calculations required the use of a computational approach beyond the usual scalar relativistic formalism and the proper account of the spin-orbit coupling in the noncollinear mode turned out to be crucial.

☎ + 421 2 602 96 551 Fax: + 421 2 602 96 231 ✉ bucko19@uniba.sk

COMENIUS UNIVERSITY IN BRATISLAVA
FACULTY OF NATURAL SCIENCES
DEPARTMENT OF PHYSICAL AND THEORETICAL CHEMISTRY
Ilkovičova 6, 842 15 Bratislava 4, Slovakia

Another major subject discussed in the thesis is the imprinting magnetism in graphene via doping and functionalization. This topic was explored in a series of studies combining experiment with simulations and the author's invaluable role in this research was to provide an atomistic level interpretation of the measured data. In the related series of papers, all being published in highly prestigious journals such as Nature Communications or JACS, the author not only proved his high scientific erudition but he also demonstrated his ability to participate in a larger multidisciplinary team in a useful way. The invitation to coauthor the review paper "Emerging chemical strategies for imprinting magnetism in graphene and related 2D materials for spintronics and biomedical applications" published in Chemical Society Reviews is in itself a recognition of Dr. Błoński's excellent scientific reputation.

Altogether, Dr. Błoński has shown in his habilitation thesis that he is an outstanding scholar who has made a number of important advances to the field of nanomagnetism. I therefore strongly support acceptance of his habilitation thesis.

Sincerely Yours,

Tomáš Bučko

☎ + 421 2 602 96 551 Fax: + 421 2 602 96 231 ✉ bucko19@uniba.sk