STATEMENT

from Dr. Sergio Madurga

(Physical Chemistry Department, Barcelona University (UB), Spain)

for the PhD work of *Miroslava Nedyalkova*

entitle *"Computational study of nanoparticles: the effect of metal ions, solvent and citric acid"*

The presented work of Miroslava Nedyalkova is a study that combines different aspects in the field of computational chemistry: Theory about colloidal stability, molecular dynamics simulations of model colloidal systems, stability of gold clusters, and conformational analysis of flexible stabilizers.

One of the main contributions of the work is the analysis of the EDL of a spherical charged nanoparticle in different salts solutions. The EDL of spherical nanoparticles has been previously studied using hard and impenetrable models of nanoparticles. However, this study is the first to analyze the role of ions in contact with a soft nanoparticle. In addition, she studied for the first time the water permeability properties for this soft nanoparticle model. Important differences between solutions of monovalent and divalent ions were identified by molecular dynamics simulations. With respect to gas phase adsorption to gold crystal nanoparticles, she identified different preferable adsorptions sites for sodium and calcium. And with respect to the conformational analysis of citrate, she carried out an *ab initio* study to analyze the coupling between conformational geometries and protonation steps that is not straightforward to obtain by experimental determination.

This work started in 2010 when Miroslava came to Barcelona thanks to a HPC grant. From this date, she has worked in the group of Biophysical chemistry of macromolecules and colloids (Biophyschem) of the Physical Chemistry Department at the Chemistry Faculty of the University of Barcelona.
On September of 2012, the procedure for developing the PhD project was open for this department.

The work presented by Miroslava shows a wide range of computational techniques used to study the main factors that are key in the description of colloidal stability.

For the development of the work, it has been very useful the three grants that Miroslava received from the HPC-Europa2 project that allow Miroslava to come to Barcelona for several months during the years 2010, 2011 and 2012. Also, the participation in the Erasmus calls and in different projects in the University of Sofia has allow to Miroslava to visit and to work physically with my group in Barcelona during the last year.
The work performed in these years has been communicated in different international congresses:

- Transnational Access Meeting (2011) in Barcelona,
- WATOC Congress (2011) in Santiago de Compostela (Spain),
- International Workshop on Nanoscience & Nanotechnology (2012) in Sofia.
- ESPA Congress (2012) in Barcelona.
- ECIS Congress (2013) in Sofia.
- International Workshop on Nanoscience & Nanotechnology (2013) in Sofia.

I want to highly, that Miroslava has been awarded in several congresses as in WATOC and in Nanoscience & Nanotechnology workshop. Also, I want to say that because of the quantity and quality of the work performed in the context of the HPC-Europa2 program, Miroslava has been invited to give an oral communication in the Transnational Access Meeting in 2012 in Amsterdam. In addition, the main part of the results of the Thesis was also communicated in the Department of Physical Chemistry of UB in the seminars of the Institute of Theoretical and Computational Chemistry (IQTCUB) in February of 2013.

With respect to communications in journals, she has three short communications in the journal of the HPC-Europa2 based on the topic of this work. And one publication, in 2012 in *The Journal of Chemical Physics.* This is an international journal with an impact factor of 3.2.

Thus, she has learned to use Molecular Dynamics simulations to analyze the role of the ions of the electric double layer, and the role of water molecules in the permeability properties of the colloid. On the other hand, the stability and structure of small gold cluster has been studied by Miroslava by means of DFT calculations. The differential adsorption of ions over the gold surface is also analyzed. And finally, she performed a systematic study of an important stabilized of gold nanoparticles. She determined the relation between conformation and protonation for the citric acid, and determine the difference between the different carboxylic groups.

Thus, the work performed by Miroslava in the PhD project certifies that she has learned to use a variety of computational techniques useful to study colloidal stability, from *ab initio* first principles to classical molecular mechanism, and now she is able to apply these computational techniques to study any particular nanoparticle of interest.

Barcelona, 24th February of 2014

Name:

Dr. Sergio Madurga