

# CV



Miroslava Aleksandrova Nedyalkova

## PERSONAL DATA

*Family name: Nedyalkova      Forename: Miroslava*  
*Date of birth : March 2nd, 1982      Gender: female*  
*Nationality: bulgarian*

## HIGHER EDUCATION AND PROFESSIONAL EXPERIENCE

### A. Academic training

<u>University degree</u>	<u>Centre</u>	<u>Date obtained</u>
BSc - Diploma in Chemistry and Physics	University of Sofia "St. Kliment Ohridsky", Faculty of Chemistry	07/2004
MSc – Diploma in "Pharmacological and medical biophysicalchemistry"	University of Sofia "St. Kliment Ohridsky", Faculty of Chemistry	25/02/2005
Doctorate	Centre	Date obtained
Theoretical and computational chemistry	University of Sofia/University Barcelona	24/03/2014

### B. Scientific or professional activities

Status/post	Institution	Period
1. Research Scientist	1. Research Sector, University of Sofia, Sofia, Bulgaria	1. 07.2007 -04.2008
2. Assistant Professor	2. University of Sofia, Sofia, Bulgaria	2. 11.2008 – 2016
3. Ph.D.	3. University of Sofia, Sofia, Bulgaria / University Barcelona	09.2011 -24.03.2014
4. Head Assistant Professor	4. University of Sofia, Sofia, Bulgaria	10.2016 -

### C. PhD thesis

**Title: Computational study of nanoparticles: effect of metal ions, solvent and citric acid.**

**Supervisor: Dr. Sergio Madurga**

**University:** University of Sofia / University of Barcelona

**Department:** Department of Inorganic Chemistry

**Date of defence of thesis:** 24/03/2014

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## STAYS IN INTERNATIONALLY RECOGNIZED CENTRES

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1. CENTRE: Faculty of Chemistry, University of Barcelona

PLACE: Barcelona COUNTRY: Spain

PERIOD: 17/05/2010 - 17/07/2010 LENGHT: 2 months

TOPIC: Overcharging of colloids – molecular dynamics study

GRANT: HPC Europe

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2. CENTRE: Faculty of Chemistry, University of Barcelona

PLACE: Barcelona COUNTRY: Spain

PERIOD: 02/2011 – 05/2011 LENGHT: 3 months

TOPIC: The effect of trivalent ions on the electrostatic properties of a charge spherical colloid - molecular dynamics study

GRANT: HPC Europe

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3. CENTRE: Faculty of Chemistry, University of Barcelona

PLACE: Barcelona COUNTRY: Spain

PERIOD: 04/2012 – 08/2012 LENGHT: 4 month

TOPIC: Adsorption of metal ions on gold nanoparticles

GRANT: HPC Europe / “ Science and business” – mobility program for young scientist – Monastery of Education and Science, Bulgaria

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4. CENTRE: Faculty of Chemistry, University of Barcelona

PLACE: Barcelona COUNTRY: Spain

PERIOD: 15/02/2013 – 15/03/2013 LENGHT: 1 month

TOPIC: Molecular dynamics simulation of a soft nanoparticle – analyzing the effect of ions on the surface of nanoparticle

GRANT: ERASMUS +

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5. CENTRE: Faculty of Chemistry, University of Barcelona

PLACE: Barcelona COUNTRY: Spain

PERIOD: 15/07/2014 – 15/10/2014 LENGHT: 3 months

TOPIC: Conformational study of citric acids like a function of pH.

GRANT: local group project

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6. CENTRE: *Laboratoire de Physico-Chimie Théorique, ESPCI*

PLACE: Paris COUNTRY: France

PERIOD: 20/07/2015 – 20/08/2015 LENGHT: 1 month

TOPIC: Monolayer of hexadecylaniline - analytical and computational approach (starting collaboration)

GRANT: FP7 – BeyondEverest project, coordinator: Sofia University

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7. CENTRE: Faculty of Chemistry, University of Barcelona

PLACE: Barcelona COUNTRY: Spain

PERIOD: 18/04/2015 – 28/04/2015 LENGHT: 10 days

TOPIC: MD study of gold clusters (preliminary tests)

GRANT: ERASMUS +

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7. CENTRE: Faculty of Chemistry, Unige

PLACE: Geneva COUNTRY: Switzerland

PERIOD: 19/05/2015 – 22/05/2015 LENGHT: 4 days

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8. CENTRE: Faculty of Chemistry, University of Barcelona

PLACE: Barcelona COUNTRY: Spain

PERIOD: 7/11/2016 – 05/12/2016 LENGHT: 28 days

TOPIC: CPMD study of carboxylic acids – pKa models (preliminary tests)

GRANT: project H20202 - TWINNING

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9. CENTRE: Faculty of Chemistry, University of Barcelona

PLACE: Barcelona COUNTRY: Spain

PERIOD: 7/02/2017 – 22/03/2017 LENGHT: 43 days

TOPIC: CPMD study of carboxylic acids – pKa models

GRANT: project H20202 - TWINNING

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10. CENTRE: Institute of Material Science, TU - Vienna

PLACE: Vienna COUNTRY: Austria

PERIOD: 22/04/2017 – 29/04/2017 LENGHT: 7 days

TOPIC: Wien2k – training

GRANT: STMS COST MP1306

## ATTENDANCES TO CONGRESSES AND CONFERENCES

### Invited lectures and seminars

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1. Second Humboldt Conference on Computational Chemistry, Nessebar 1-5 Sept. 2004
2. IV National conference for students 18-20.05.2005 Sofia Bulgaria
3. Centre Européen de Calcul Atomique et Moléculaire, France, Lyon, CP/MD- Molecular simulations, 07-18.11.2005
4. V National conference for students 17-19.05.2006 Sofia Bulgaria
5. ICN+T 2006 NANAO09 MEETS STM06, 31.07-4.08.2006, Basel, Switzerland
6. ICTP/Democritus Joint Workshop "Tools for Computational Physics", 6-11.03.2006., Trieste, Italy
7. 13th International Workshop NANOSCIENCE & NANOTECHNOLOGY , 2011, Sofia , Bulgaria, **November 25-26, 2011**
8. 7<sup>th</sup> National Conference of Chemistry. International Conference on Green Technologies and Environmental Protection, 26.05-29.05.2011, Sofia, Bulgaria,
  1. 08 – 09. 06. 2011 - TAM (Transnational Access Meeting) of the HPC-Europa2 project, organized by Mare Nostrum in Barcelona
  2. 22-23 November 2012: Technical University of Sofia, Bulgaria, NANO'2012
  3. 17-22.07.2011 WATOC, Santiago de Compostella, Spain - <http://www.watoc2011.com/index.php/home>
  4. ESPA 2012, Barcelona, Spain
  5. 22.06.2012- TAM (Transnational Access Meeting) of the HPC-Europa2 project, organized by SARA in Amsterdam - **invited**

6. ECIS 2013: 27th Conference of the European Colloid and Interface Society, September 01–06, 2013, Sofia, Bulgaria - <http://www.ecis-web.eu/abstracts/sofia2013/Program-ECIS-2013-Sofia.pdf>
  7. 14 - 17.04.2014 - Emergent Colloidal Dynamics Far From Equilibrium, CECAM, EPFL, Lausanne, Switzerland
  8. 25-27 June 2014, Superhydrophobicity, bubble stability and heterogeneous nucleation, Rome, Workshop - <http://www.dima.uniroma1.it/dima/superhydrophobicity2014>
  9. 16<sup>th</sup> International Workshop on Nanoscience and Nanotechnology, NANO 2014, 7 - 8 November 2014, Sofia
  10. 07.02 – 14.02.2015 - Workshop at University Torino, group of prof. M.Barico, - oral presentation – **invited**
  11. 26.06 – 1.07.2016 – Multiple scattering codes, Rennes, COST Action 1306, France
  12. 5.09-9.09.2016 – TNT 2016, Fribourg, Switzerland
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## **OTHER ACHIEVEMENTS AND ACTIVITIES**

### **Grants and others fellowships received**

2005 Fellowship for 6 months from Swiss Government for excellent results as undergraduate student

2010 – 2012 – HPC2EUROPE – 3 grants, University Barcelona, Faculty of Chemistry

2013 – Science and business – Bulgarian Ministry of Education, travel grants for young scientist – host University of Barcelona, Faculty of Chemistry

2011 Award for young scientists - WATOC conference - BEST POSTER

2013 Award Nanoscience and Nanotechnology conference – Bulgaria, BEST POSTER

2013 – 2016 ERASMUS teaching grants – UB, Barcelona

2014 Award Nanoscience and Nanotechnology - Bulgaria, BEST POSTER

### **Organization of conferences and projects**

Member of the organizing committee of the following events:

1. Conferences for E- learning methods, 10/2014, Sofia, Bulgaria

2. Conferences for E- learning platform in Faculty of Chemistry and Pharmacy, 12/2014, Sofia, Bulgaria

3. Main coordinator in project- "E-learning forms in Faculty of Chemistry and Pharmacy"- Human Resource Development, **BG051PO001-4.3.04-0033**

4. Advisor for a work package in project- "Build a teams of young scientists in the field of biomedical research areas", Human Resource Development, **BG051PO001-3.3.04-0040**
5. Organization of 10 local discussion seminars for young scientist in the chemistry, physics and medicine research – 2012 – 2014
6. Conference organization committee – "Build a teams of young scientists in the field of biomedical research areas", 21 – 27/11/2013, Pravetz, Bulgaria
7. Management Committee - BULGARIA – COST – MP1306 – EUSpec
8. COST Action IS1408
9. Funding grant – DCOST 2016/18 – FNI – Bulgaria – 24 months

### **PRESENT RESEARCH AREA**

*Brief summary (key words).*

Computational chemistry, molecular dynamic, metal clusters, metal surfaces, nanoparticles, adsorption, monolayers, multivariate statistics

1. Theory of tip-dependent imaging of adsorbates in the STM: CO on Cu(111)Drakova, M. Nedjalkova, G. Doyen, Volume 106 Issue 6, Pp.1419-1431 International Journal of Quantum Chemistry;
2. Overcharging of colloids, Science and Supercomputing in Europe; Research Highlights 2010, HPC-Europa2 Report 2010, Ed Miroslava Nedyalkova, CINECA Consorzio Interuniversitario, Bologna (2010) p.35.;
3. Overcharging of colloids-part 2, Science and Supercomputing in Europe; Research Highlights 2011, HPC-Europa2 Report 2010, Ed. Miroslava Nedyalkova, CINECA Consorzio Interuniversitario, Bologna (2011);
4. The effect of trivalent ions on the electrostatic properties of a charge spherical colloid: Molecular dynamic study with explicit wate molecules, Nanoscience & Nanotechnology, 12 eds. E. Balabanova, E. Mileva, Sofia, 2012;
5. Molecular dynamics simulation of the spherical electrical double layer of a soft nanoparticle: effect of the surface charge and counterion valence., Nedyalkova M, Madurga S, Pisov S, Pastor I, Vilaseca E, Mas F., J Chem Phys. 2012 Nov 7;137(17):174701;
6. Adsorbtion of metal ions on gold nanoparticles, HPC-Europa2 Report 2010, Ed. Miroslava Nedyalkova, CINECA Consorzio Interuniversitario, Bologna (2012);
7. Preparation and characterization of PVA/PEG/Boron Hybrid materials, H.Hristov, P.Vasileva, M.Nedyalkova, Nanoscience & Nanotechnology,12 eds. E. Balabanova, E. Mileva, Sofia, 2012;
8. Formation of platinum nanoparticles by the spontaneous reduction of hexadecylanilinelangmuir monolayers at air-water surface, M.Nedyalkova,

H.Hristov, Nanoscience & Nanotechnology, 12 eds. E. Balabanova, E. Mileva, Sofia, 2012;

9. Принципите на ефективното електронно обучение във Факултета по химия и фармация на СУ. Мирослава Недялкова, Стефан Цаковски, Васил Симонов, Списание „Наука“ бр. 1, 2015
10. Solid State Structure Prediction Through DFT Calculations and <sup>13</sup>CNMR Measurements: Case Study of Spiro-2,4-dithiohydantoin, Vladislav Antonov, Miroslava Nedyalkova, Pavleta Tzvetkova, and Anife Ahmedova, Zeitschrift für Physikalische Chemie, DOI:10.1515/zpch-2015-0710;
11. The Boron Oxide Glasses and Nanocomposites: Synthetic, Structural and Statistical Approach, Hr. Hristov, M. Nedyalkova, V.Simeonov, Journal of Materials Science & Technology (<http://dx.doi.org/10.1016/j.jmst.2016.07.016>);
12. Modeling of pharmaceuticals mixtures toxicity with deviation ratio and best-fit functions models, Monika Wiczerzak, Błażej Kudlak, Galina Yotova, Miroslava Nedyalkova, Stefan Tsakovski, Vasil Simeonov, Jacek Namieśnik, The Science of the total environment. (Sci. Total Environ.). 571: 259-68,
13. Chemometric expertise of the ecotoxicity/physicochemical features links of silver nanoparticles - environmental aspects, M. Nedyalkova, B. Donkova, V.Simeonov, JAOACS - vol.100, No.2, 2017;
14. Statistical approach to study of lithium magnesium metaborate glasses – M. Nedyalkova, Hr. Hristov, V.Simeonov - Open Chem., 2017; 15: 1–6;
15. Insight into electric field-induced rupture mechanism of water-in-toluene emulsion films from a model system, Dessislava Dimova, Stoyan Pisov, Nikolay Panchev, Miroslava Nedyalkova, Sergio Madurga, and Ana Proykova, *Journal of Chemical Physics*, 2017, (just accepted) ;
16. Multivariate statistical classification of plant features – the case with *Onobrychis pindicola* Subsp. *urumovii* Degen & Dren.- Comptes rendus de l'Académie bulgare des Sciences., 2017, (accepted)
17. Interface properties of iron oxide nanoparticles: from computational design to biomedical application - M.Nedyalkova, S.Madurga, V. Simeonov - *Advances in Colloid and Interface Science Journal*: (DOI information: 10.1016/j.cis.2017.05.003)
18. Application of chemometric techniques in studies of toxicity of selected commercially available products for infants and children, Environmental Monitoring and Assessment (just accepted)