

Curriculum Vitae

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Education

Organic Chemistry, Department of Organic Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia

Honors

Doctor of Philosophy, Organic Chemistry/Chemical Physics, Department of Organic Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia, February 2006

Master of Science, Organic Chemistry, Department of Organic Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia, 2001

Principal scientific activities

current:

- Atomistic molecular dynamics (MD) simulations of synthetic biocompatible polymers grafted onto solid surfaces focused on the structure and properties of grafted chains as well as on investigation of characteristic features of thus modified surfaces.
- Atomistic MD simulations of surfaces covered by layers of anchored polymers as potential barrier against undesired protein adsorption
- Atomistic MD simulations of wetting properties of surfaces covered by irreversibly anchored polymers immersed in the matrix of free chemically identical polymers
- Coarse-grained Metropolis Monte Carlo simulations of linear and cyclic chains of different stiffness under uni-, bi-, and triaxial confinements modeling biomacromolecular systems (DNA, actin) focused on structural properties and scaling relationships of these properties influenced by confinement

previous:

- Quantum-chemical calculations of the electric properties of organic molecules associated with the nonlinear optical properties using variety of theoretical approaches
- Teaching activities: Faculty of Natural Sciences, Comenius University, 2002-2003
- Seminars on organic chemistry
 - Exercises on organic chemistry
 - Exercises on laboratory methods
 - Seminars on molecular modeling

Participation in projects

1. „**Protection of surfaces against protein adsorption: poly(ethylene oxide) vs poly(oxazoline)**”, 2020-2023, principal investigator, VEGA
2. „**Interactions of surfaces modified by poly(ethylene oxide) with free polymers**”, 2016-2019, principal investigator, VEGA
3. „**Structural transitions of (bio)macromolecules in nanochannels**”, 2016-2019, participating investigator, APVV
4. „**Nanostructure of (bio)macromolecular systems in nanochannels**”, 2016-2019, participating investigator, VEGA
5. „**Safety and Quality of Food of Nanotechnology**”, 09/2016-04/2018, participating investigator, FEDER
6. „**Molecular Dynamics Simulations of PEO-Modified Surfaces Immersed in a Matrix of Homopolymer Melts or Solutions**”, 04/2013-09/2016, principal investigator, Foundation for Science and Technology, Portugal
7. „**Molecular dynamics simulations of tethered PEO layers as potential barriers to protein adhesion**”, 2010-2013, principal investigator, Foundation for Science and Technology, Portugal
8. „**Structural transitions of confined semiflexible macromolecules**“, 2012-2015, participating investigator, VEGA
9. „**Nanostructure in macromolecular systems induced by confinement**“, 2012-2015, participating investigator, APVV
10. „**Quantification of geometrically confined macromolecules in polymeric materials and processes**“, 2008-2010, participating investigator, APVV
11. „**Properties and utilization of semiflexible (bio)macromolecules confined in microchannels and micropores**“, „**Vlastnosti a využitie menej ohybných (bio)makromolekul uväznených v mikrokanáloch a mikropóroch**“, 2009-2011, participating investigator, VEGA
12. „**Nanoscale simulations of (bio)macromolecular systems with special and phase interfaces**“, „**Nanoškálové simulácie (bio)makromolekulových systémov s priestorovými a fázovými rozhraniami**“, 2006-2008, participating investigator, VEGA
13. „**Advanced computational chemistry, CE SAV COMCHEM**”, 2007-2010, participating investigator, Centrum of Excellence
14. „**Semiflexible filamentous actin chain in biaxial confinement of microchannel**”, 2007, principal investigator, Polymer Institute, Slovak Academy of Sciences
15. „**Structure-nonlinear optical properties relationship of organic molecules**”, 2005, principal investigator, Comenius University
16. „**Theoretical study of nonlinear optical properties for organic molecules**”, 2003, principal investigator, Comenius University

Funding ID

1. VEGA 2/0098/16

2. SRDA-15-0323
3. VEGA 2/0055/16
4. NORTE-01-0415-FEDER-000011
5. SFRH/BPD/90265/2012
6. SFRH/BPD/63568/2009
7. 2/0093/12, VEGA
8. APVV-0451-11
9. APVV-0079-07
10. VEGA 2/0144/09
11. VEGA 2/6014/26
12. COMCHEM
13. 1224 Polymer Institute, Slovak Academy of Sciences
14. UK-125-2005
15. UK-125-2003

Achievement-Track Record

- Winner of **Š. Schwarz Fund** support of SAS for the 10 best PhD theses (2006-2010)
- Award of the junior researcher (till the age of 35 years) for the best work in 2012 at the Polymer Institute, Slovak Academy of Sciences
- Principal investigator of two international and three national projects
- 27 publications in CC journals
- Participation in international scientific conferences (talks, poster presentations)
- ~320 SCI/WOS citations

Research expeditions

3-year stay at the Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Portugal, Supervisor: Prof. M. Natália D. S. Cordeiro February 2010-January 2013

3-month visiting research stay at the Department of Chemistry, Faculty of Science, Catholic University of Leuven, Belgium, Supervisor: Prof. Erik Nies, 2008

2-month visiting research stay at the Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic in Prague, Czech Republic, Supervisor: Prof. M. Lísal, 2007

10-month visiting study stay at the Department of Quantum Chemistry, Institute of Chemistry, Nicolaus Copernicus University of Torun, Poland, Supervisor: Prof. A. J. Sadlej, 2003-2004

2-month visiting study stay at the Department of Organic Chemistry, Institute of Chemistry, Karl-Franzens University of Graz, Austria, Supervisor: Prof. W. M. F. Fabian, 2003

2-month visiting study stay at the Department of Organic Chemistry, Institute of Chemistry, Karl-Franzens University of Graz, Austria, Supervisor: Prof. W. M. F. Fabian, 2002