

ANNA V. GUBSKAYA

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Homepage: <http://biocomputations.org/>

OBJECTIVE: A leading research position in a computational group of a company specializing in development of novel pharmaceuticals, biomedical products or biomaterials

PROFESSIONAL INTERESTS

- Atomistic simulations of biologically relevant compounds/systems
- QSAR/QSPR modeling in drug discovery and material science
- Computer-aided design of virtual combinatorial libraries

HIGHLIGHTS OF QUALIFICATIONS

Computational Chemistry:

- Proficient in *ab initio*, molecular dynamics and molecular mechanics computer simulations and applications of machine-learning algorithms: decision trees, artificial neural networks (ANN) and polynomial neural networks (PNN)
- Experienced in utilization of corresponding state-of-art commercial and free-distributed simulation packages on Unix, Linux, SGI, Windows and MacOS platforms such as Gaussian, Cerius2, Materials Studio, Molecular Operating Environment (MOE), MacroModel, HyperChem, CHARMM, DL-POLY, MDynaMix, WEKA

Experimental Physics / Chemistry:

- Extensive experience in IR spectroscopy, mass spectrometry and X-ray diffraction methods

Languages: Fluent in Russian, Ukrainian, English and literate in French

EDUCATION

Doctor of Philosophy - Chemistry	2003
Dalhousie University, Halifax, NS, Canada (2000-2003)	
<i>Advisor:</i> Prof. P.G. Kusalik	
Master of Science - Chemistry	2000
Dalhousie University, Halifax, NS, Canada (1998-2000)	
<i>Advisor:</i> Prof. P.G. Kusalik	
Doctor of Philosophy - Physics & Mathematics	1993
B. Verkin Institute for Low Temperature Physics and Engineering (ILTPE)	
Ukrainian National Academy of Science (UNAS), Kharkov, Ukraine (1988-1993)	
Master of Science (Bachelor of Science integrated) - Biophysics	1981
V. Karazin Kharkov National University, School of Radiophysics,	
Department of Molecular Biophysics, Kharkov, Ukraine (1976-1981)	
University Diploma of Art Critic	1981
V. Karazin Kharkov National University, School of Community Professions	
(3 year program), Kharkov, Ukraine	

EMPLOYMENT AND RELATED EXPERIENCE

Research Associate 2007-2008
New Jersey Center for Biomaterials / Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, USA

Leader of the projects: "Prediction of bioresponse for large combinatorial libraries of polymethacrylates", "Computational modeling and prediction of polymeric drug release".

Personal contribution: molecular modeling and computer-aided combinatorial design, molecular dynamics simulations.

Post-doctoral Research Associate 2005-2007
New Jersey Center for Biomaterials / Department of Mechanical and Aerospace Engineering,
Rutgers University, Piscataway, NJ, USA

Leader of the project: "Computational modeling and prediction of polymeric drug delivery using logical analysis of data (LAD) method".

Personal contribution: development of combined molecular dynamics and semi-empirical modeling approach for polyarylates, computer-aided design of virtual combinatorial libraries of polymethacrylates and poly(β -amino esters).

Post-doctoral Fellow 2003-2005
Department of Chemistry, Dalhousie University, Halifax, Canada

Personal contribution: molecular modeling / computer simulations of potassium ion channel and amyloid- β peptide associated with Alzheimer's disease.

Graduate Assistant 1998-2003
Department of Chemistry, Dalhousie University, Halifax, Canada

Graduate research: *ab initio* and molecular dynamics computational studies of strongly associated liquids.

Senior Research Associate 1997-2001
Special Engineering Bureau of ILTPE, Kharkov, Ukraine

Personal contribution: scientific consultant / principal investigator on the project related to applications and development of cryogenic technologies for pharmaceutical industry.

Senior Research Associate 1996-1997
Department of Molecular Modeling, I. Mechnikov Scientific Research Institute for Microbiology and Immunology, Kharkov, Ukraine

Personal contribution: principal investigator in computational studies and computer-aided design of antimicrobial compounds.

Junior Research Associate 1989-1996
Department of Molecular Biophysics, ILTPE, Kharkov, Ukraine

Personal contribution: experimental (UR, mass-spectrometry, X-ray diffraction) studies of molecular crystals (drugs).

Engineer / Research Assistant 1981-1989
Department of Molecular Biophysics, ILTPE, Kharkov, Ukraine)

Personal contribution: spectroscopic (UV, IR) studies of selected biomolecules.

ADDITIONAL WORK EXPERIENCE

Teaching Assistant 1998-2003
Department of Chemistry & Dalhousie Integrated Science Program (DISP), Dalhousie University, Halifax, Canada)

- Assisted students in their laboratory and home work, evaluation of their performance

Mentorship 2005-2008
New Jersey Center for Biomaterials, Rutgers University, Piscataway, NJ, USA

- Mentored graduate students of NJCBM and supervised Senior Design Projects of undergraduate students from the Department of Biomedical Engineering, Rutgers University.

Acting Manager 2007-2008
New Jersey Center for Biomaterials, Rutgers University, Piscataway, NJ, USA

- Managed the project on synthesis, characterization and computational modeling of combinatorial library of polymethacrylates

Reviewer of manuscripts for scientific journals: Australian Journal for Chemistry, Polymer.

PRESENTED AT CONFERENCES

- 2007 16-th Canadian Symposium on Theoretical Chemistry (St. John's, NL, Canada)
2007 90-th Canadian Chemistry Conference and Exhibition, invited speaker for the symposium on Biocomputational Chemistry (Winnipeg, MN, Canada)
2006 8-th Symposium on Biomaterials Science (New Brunswick, NJ, USA)
2006 6-th Canadian Computational Chemistry Conference, (Vancouver, BC, Canada)
2006 89-th Canadian Chemistry Conference and Exhibition (Halifax, NS, Canada)
2006 Society for Biomaterials Annual Meeting (Pittsburgh, PA, USA)
2004 15-th Canadian Symposium on Theoretical Chemistry (Québec, Canada)
2000 16-th IUPAC Conference on Chemical Thermodynamics (Halifax, NS, Canada)
1996 NATO ASI Summer School on Crystal Engineering (Digby, NS, Canada)
1996 7-th College on Biophysics: Structure and Function of Biopolymers (Trieste, Italy)
1996 12-th Conference in Coordinational and Supramolecular Chemistry (Chishinau, Moldova)
1995 International Conference in Microbiology and Immunology (Kharkov, Ukraine)
1994 International conference on Powder Diffraction and Crystal Chemistry (St. Petersburg, Russia)
1991 5-th All-Union Conference in Low Temperature Chemistry (Moscow, USSR)
1988 International Conference in Cryobiology and Cryomedicine (Kharkov, USSR)
1986, 1989, 1990, 1991 18-th, 20-th, 21-th, 22-th Conferences of Young Scientists (ILTPE, Kharkov, USSR)
1982 1-st All-Union Biophysical Congress (Moscow, USSR)

ACHIEVEMENTS, GRANTS, AWARDS

- 2007 Invited speaker at the 90th Canadian Chemistry Conference and Exhibition, May 26-30, 2007, Winnipeg, MN, Canada
2001 Invited visitor in Division of Physical Chemistry, Arrhenius Laboratory of Stockholm University (Stockholm, Sweden)
1997 The academic rank of Senior Research Associate in Biophysics was awarded and certified by Higher Certifying Board of the Ukraine
1997 Ukrainian State Foundation for Fundamental Investigations, Long-Term Research Grant (Principal Investigator)
1996 NATO travel grant to participate in NATO ASI Summer School on Crystal Engineering (Digby, NS, Canada)
1996 Travel award from International Center for Theoretical Physics (ICTP), Italy to attend the 7-th College on Biophysics: Structure and Function of Biopolymers
1994 International Science Foundation (ISF), Long-Term Research Grant (U2J000)
1993 ISF, Long-Term Research Grant (U2J200)

PROFESSIONAL MEMBERSHIP

- Since 2004 Member, American Chemical Society
Since 1999 Member, Chemical Institute of Canada

SELECTED PUBLICATIONS

BOOK CHAPTERS

A.V. Gubskaya

Quantum-Chemical Descriptors in QSAR Modeling: Achievements, Trends and Perspectives. In *Quantum Biochemistry: Electronic Structure and Biological Activity*. Editor: C.F. Matta, Wiley-VCH, Weinheim (to be released by the end of 2009).

A.V. Gubskaya and P.G. Kusalik

A mean-field approach for the determination of the polarizabilities for the water molecule in liquid state. In *Computational Aspects of Electric Polarizability Calculations: Atoms, Molecules and Clusters*. Editor: G. Maroulis, 2006, Amsterdam: IOS Press Inc., 536 p.

PEER-REVIEWED ARTICLES

V. Kholodovych, A.V. Gubskaya, M. Bohrer, N. Harris, D. Knight, J. Kohn, W.J. Welsh
Prediction of Biological Response for Large Combinatorial Libraries of Biodegradable Polymers: Polymethacrylates as a Test Case. *Polymer*, 2008, **49**, 2435-2439.

A.V. Gubskaya, V. Kholodovych, D. Knight, J. Kohn, W.J. Welsh

Prediction of Fibrinogen Adsorption for Biodegradable Polymers: Integration of Molecular Dynamics and Surrogate Modeling. *Polymer*, 2007, **48**, pp. 5788-5801.

Yu. V. Lisnyak, A.V. Martinov, V.N. Baumer, O.V. Shishkin, A.V. Gubskaya
Crystal and Molecular Structure of β -Cyclodextrin Inclusion Complex with Succinic Acid. *J. Inclusion. Phenom. Macrocyclic Chem.*, 2007, **58**, pp. 367-375.

A.V. Gubskaya and P.G. Kusalik

Molecular dynamics simulation study of ethylene glycole, ethylenediamine and 2-aminoethanol. 2. Structure in aqueous solutions. *J. Phys. Chem.*, 2004, **108**(35), pp. 7165-7176.

A.V. Gubskaya and P.G. Kusalik

Molecular dynamics simulation study of ethylene glycole, ethylenediamine and 2-aminoethanol. 1. The local structure in pure liquids. *J. Phys. Chem.*, 2004, **108**(35), pp. 7151-7164.

Yu.V. Lisnyak, M.V. Kosevich, A.V. Gubskaya

Conformational possibilities of a glycerol molecule. *Bulletin of Kharkov State University*, 2004, N637, Issue 1-2 (14), pp.5-15 (in Russian).

A.V. Gubskaya and P.G. Kusalik

Mean-field method in determination of the molecular polarizabilities for the water molecule in liquid state. *JCMSE (Journal of Computational Methods in Sciences and Engineering)* 2004, **4**(4) pp. 641-664.

A.V. Gubskaya and P.G. Kusalik

The total molecular dipole moment for liquid water. *J. Chem. Phys.*, 2002, **117**(11), pp. 5290-5302.

A.V. Gubskaya and P.G. Kusalik

The multipole polarizabilities and hyperpolarizabilities of the water in liquid state: *ab initio* study. *Mol. Phys.*, 2001, **90**, pp.1107-1120.

A.V. Gubskaya, S.A. Aksyonov, A.N. Kalinkevich, Yu.V. Lisnyak, V.P. Chuev, V.D. Chivanov
²⁵²Cf Plasma Desorption Mass Spectrometric Study of the Inclusion Complexes of Cyclodextrines with Coumarines. *Rapid Communications in Mass Spectrometry*, 1997, **11**, pp.1874-1878.

A.V. Gubskaya, K.A. Chishko, Yu.V. Lisnyak, Yu.P. Blagoy

Effect of Cryogrinding on Physico-Chemical Properties of Drugs. II. Cortisone Acetate: Particles Sizes and Polymorphic Transition. *Drug Development and Industrial Pharmacy*, 1995, **21**(17), pp. 1965-1974.

A.V. Gubskaya, Yu.V. Lisnyak, Yu.P. Blagoy

Effect of Cryogrinding on Physico-Chemical Properties of Drugs. I. Theophylline: Evaluation of Particles Sizes and the Degree of Crystallinity, Relation to Dissolution Parameters. *Drug Development and Industrial Pharmacy*, 1995, **21**(17), pp. 1953-1964.

A.V. Gubskaya, O.A. Boryak, M.V. Kosevich, V.S. Shelkovsky, Yu.P. Blagoy

Sensitivity of FAB Mass Spectrometry to Various Polymorphic Forms of Cortisone Acetate. *Rapid Communications in Mass Spectrometry*, 1992, **6**, pp. 531-535.

A.V. Gubskaya, Yu.V. Lisnyak, V.G. Khomenko, Yu.V. Telezhenko, L.F. Sukhodub, Yu.P.

Blagoy Morphological and Structural Characteristics of Cryogrinded Cortisone Acetate. *Doklady Akademii Nauk Ukrainy (Proceedings of Academy of Sciences of Ukrainian SSR)*, 1992, N12, pp.86-89 (in Russian).

B.I. Verkin, A.V. Gubskaya, Yu.V. Lisnyak, Yu.A. Pokhyl, V.G. Khomenko, L.F. Sukhodub

Effect of Cryogrinding on Structural Characteristics of Theophylline. *Doklady Akademii Nauk SSSR (Proceedings of Academy of Sciences of USSR)*, 1988, **301**(5), pp.1128-1131 (in Russian).

V.G. Khomenko, A.V. Gubskaya, V.V. Mitkevich, Yu.V. Telezhenko, L.F. Sukhodub

Structure, Thermal Expansion of Theophylline and Theobromine Crystals and Hydrogen Bonds. *Preprint ILTPE (B.I. Verkin Institute for Low Temperature Physics and Engineering, Ukrainian Academy of Science)*, Kharkov 1988, N 6-88, pp.1-14 (in Russian).

B.I. Verkin, A.V. Gubskaya, Yu.V. Telezhenko, L.F. Sukhodub

The Cryogrinding of Medicinal Compounds (Problems, Purposes and Perspectives). *Preprint ILTPE (B.I. Verkin Institute for Low Temperature Physics and Engineering, Ukrainian Academy of Science)*, Kharkov 1986, N 57-86, pp.1-33 (in Russian).

RECENT CONFERENCE CONTRIBUTIONS

Yu. V. Lisnyak, A. V. Gubskaya

Molecular dynamics study of hydrogen bonding interactions in calcineurin inhibitor peptide-polymer model systems. The 1st International Symposium "Supramolecular and Nanochemistry: toward Applications" August 25-29, 2008, Kharkov, Ukraine.

J. Kohn, A. V. Gubskaya, V. Kholodovych, W. J. Welsh, D. Knight

New Computational Model for Prediction of Protein Adsorption on the Surfaces of Biomaterials. The 8th World Biomaterials Congress, May 28 - June 1, 2008, Amsterdam, The Netherlands.

A.V. Gubskaya, T.O. Bonates, V. Kholodovych, J. Kohn, D. Knight, W.J. Welsh

Machine-Learning Models in Computer-Aided Discovery of Biodegradable Polymers. The 16th Canadian Symposium on Theoretical Chemistry, August 4-9, 2007, St. John's, NL, Canada.

Yu.V. Lisnyak, A.V. Martynov, A.V. Gubskaya

Molecular Modeling Study of Polyene-Sterol Membrane Channel. The 2nd Symposium on Methods and Applications of Computational Chemistry, July 2-4, 2007, Kyiv, Ukraine.

A.V. Gubskaya, V. Kholodovych, D. Knight, J. Kohn, W.J. Welsh

Computer-Aided Prediction of Bioresponse for Combinatorial Libraries of Biodegradable Polymers. The 90th Canadian Chemistry Conference and Exhibition, May 26-30, 2007, Winnipeg, MN, Canada.

L.M. Valenzuela, A. Gubskaya, J. Kohn, D. Knight

Molecular Modeling of L-Tyrosine-Derived Polyarylates: Conformational Behavior Depending on Force Field. The 8th New Jersey Symposium, November 8-10, 2006, New Brunswick, NJ, USA.

V. Kholodovych, A. Gubskaya, D. Knight, W.J. Welsh

Computational Models for Predicting Biorelevant Properties of Polymethacrylates. The 8th New Jersey Symposium, November 8-10, 2006, New Brunswick, NJ, USA.

A. Gubskaya, D. Knight, J. Kohn

Prediction of Fibrinogen Adsorption onto Polymer Surfaces: 3D Case Study. The 6th Canadian Computational Chemistry Conference, July 26-30, 2006, Vancouver, BC, Canada.

A. Gubskaya, D. Knight, J. Kohn

Prediction of Fibrinogen Adsorption for the Library of Biodegradable Polyarylates: Combined Computational Modeling Approach. The 89th Canadian Chemistry Conference and Exhibition, May 27-31, 2006, Halifax, NS, Canada.

L. Valenzuela, A. Gubskaya, J. Kohn, D. Knight

Molecular Modeling and Computational Study of Tyrosine-Derived Polyarylates. Society for Biomaterials Annual Meeting, April 26-29, 2006, Pittsburgh, PA, USA.

A. Gubskaya, J. Schut, J. Kohn, D. Knight

Molecular Dynamics Simulations in Investigating the Liquid Crystalline Behavior Found in Biodegradable Polyarylates. Society for Biomaterials Annual Meeting, April 26-29, 2006, Pittsburgh, PA, USA.

A. Gubskaya, V. Kholodovych, L. M. Valenzuela, J. Kohn, D. Knight

Prediction of Fibrinogen Adsorption for the Library of Novel Biodegradable Polymers: Combined Molecular Dynamics and Surrogate Modeling Approach. Society for Biomaterials Annual Meeting, April 26-29, 2006, Pittsburgh, PA, USA.

MANUSCRIPTS IN PROGRESS

A.V. Gubskaya, T.O. Bonates, P.L. Hammer, V. Kholodovych, R. Langer, J. Kohn

Logical Analysis of Data in Structure-Property Investigation of Polymeric Gene Delivery (prepared for JBMR and transferred to J. Kohn's office for submission).

A. Gubskaya, J. Khan, L. Valenzuela, Yu. Lisnyak, J. Kohn

Experimental and computational studies of the release of a calcineurin inhibitor peptide from tyrosine-derived polycarbonate terpolymers.