

ANNA V. GUBSKAYA

Contact: 1-28 Gebhardt St.
Halifax, NS, B3M 2X1, Canada
Tel: 902-293-7498
E-mail: ggubska-at-dal.ca
ganna.gubska-at-msvu.ca
Website: <http://biocomputations.org/>

OBJECTIVE

A leading research position in a computational group of a governmental institution specializing in life sciences and/or environmental research

RESEARCH INTERESTS

- Atomistic simulations of biologically relevant compounds and molecular systems
- Cheminformatics, QSAR/QSPR modeling in drug discovery, life and material sciences
- Computer-aided design of virtual combinatorial libraries of novel molecules

HIGHLIGHTS OF QUALIFICATIONS

Theoretical and 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 such as Gaussian, Cerius2, Materials Studio, Molecular Operating Environment (MOE), MacroModel, HyperChem, CHARMM, DL-POLY, MDynaMix, WEKA on Unix, Linux, SGI, Windows, and Mac OS platforms

Experimental Physics and Physical Chemistry

- Knowledge of and practical experience in IR spectroscopy, mass spectrometry and X-ray diffraction methods

Management

- Acted as a manager on the multidisciplinary project related to synthesis, characterization and computational modeling of biodegradable polymers

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

EDUCATION

Doctor of Philosophy - Chemistry Dalhousie University, Halifax, Nova Scotia, Canada	2000-2003
Master of Science - Chemistry Dalhousie University, Halifax, Nova Scotia, Canada	1998-2000
Doctor of Philosophy - Physics & Mathematics 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 V. Karazin Kharkov National University, School of Radiophysics, Department of Molecular Biophysics, Kharkov, Ukraine	1976-1981
University Diploma of Art Critic V. Karazin Kharkov National University, School of Community Professions (3 year program), Kharkov, Ukraine	1978-1981

EMPLOYMENT AND RELATED EXPERIENCE

Visiting Research Investigator

2017-2017

College of Pharmacy, University of Michigan, Ann Arbor, MI, USA

Adjunct Professor & Instructor

2009-2012

Department of Physics and Chemistry, Mount Saint Vincent University, Halifax, NS, Canada

Remote Research Consultant

2008-2009

Department of Molecular Modeling, I. Mechnikov Scientific Research Institute for Microbiology and Immunology, Kharkov, Ukraine

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, NS, 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, NS, Canada

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

Senior Research Associate

1997-2001

Special Engineering Bureau of B. Verkin Institute for Low Temperature Physics and Engineering (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**

2009-2010, 1998-2003

- General chemistry

Department of Physics and Chemistry, Mount Saint Vincent University & Department of Chemistry, Dalhousie University, Halifax, NS, Canada

- Multidisciplinary problem solving sessions

Dalhousie Integrated Science Program (DISP), Dalhousie University, Halifax, NS, Canada

Mentorship

2005-2008

- Principles of molecular modeling

New Jersey Center for Biomaterials (graduate students) / Department of Biomedical Engineering (undergraduate students on Senior Design Projects), Rutgers University, Piscataway, NJ, USA

Acting Manager

2007-2008

New Jersey Center for Biomaterials (a project on synthesis, characterization, and computational modeling of combinatorial library of polymethacrylates), Rutgers University, Piscataway, NJ, USA

Reviewing manuscripts

Journals: Australian Journal for Chemistry, Polymer

PRESENTED AT INTERNATIONAL CONFERENCES**2007** 16-th Canadian Symposium on Theoretical Chemistry (St. John's, NL, Canada)**2007** 90-th Canadian Chemistry Conference and Exhibition (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)**1988** International Conference in Cryobiology and Cryomedicine (Kharkov, 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** The North Atlantic Treaty Organization (NATO) – travel grant to participate in NATO ASI Summer School on Crystal Engineering (Digby, NS, Canada)
- 1996** International Center for Theoretical Physics (ICTP) – travel award to attend the 7-th College on Biophysics: Structure and Function of Biopolymers (Trieste, Italy)
- 1994** International Science Foundation (ISF) – long term research grant (U2J000)
- 1993** International Science Foundation (ISF) – long term research grant (U2J200)

PROFESSIONAL MEMBERSHIP

Since 2004 – member of American Chemical Society

Since 1999 – member of 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, 2010, Wiley-VCH, Weinheim, 880p.

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

A.V. Gubskaya, I.J. Khan, L.M. Valenzuela, Y.V. Lisnyak, J. Kohn

Investigating the Release of a Hydrophobic Peptide from Matrices of Biodegradable Polymers: An Integrated Method Approach, *Polymer*, 2013, **54**, pp. 3806-3820.

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

Logical Analysis of Data in Structure-Property Investigation of Polymeric Gene Delivery. *Macromol. Theor. Simul.*, 2011, **20**, pp. 275-285.

C. F. Matta, L. Massa, A.V. Gubskaya, and E. Knoll

Can you Take the Logarithm or the Sine of a Dimension or a Unit? Dimensional Analysis Involving Transcendental Functions. *J. Chem. Educ.*, 2011, **88**, pp.67-70.

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**, pp. 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).

Selected 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 8-th 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 8-th 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.

REFERENCES AVAILABLE UPON REQUEST