ANNA V. GUBSKAYA

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OBJECTIVE

A leading research position in a computational group of a governmental institution specializing in development of novel pharmaceuticals, biomedical products or/and biomaterials

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 drugs and polymers

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 2000-**2003**
Dalhousie University, Halifax, Nova Scotia, Canada

Master of Science - Chemistry 1998-**2000**
Dalhousie University, Halifax, Nova Scotia, Canada

Doctor of Philosophy - Physics & Mathematics 1988-**1993**
B. Verkin Institute for Low Temperature Physics and Engineering (ILTPE)
Ukrainian National Academy of Science (UNAS), Kharkov, Ukraine

Master of Science (Bachelor of Science integrated) - Biophysics 1976-**1981**
V. Karazin Kharkov National University, School of Radiophysics,
Department of Molecular Biophysics, Kharkov, Ukraine

University Diploma of Art Critic 1978-**1981**
V. Karazin Kharkov National University, School of Community Professions
(3 year program), Kharkov, Ukraine

EMPLOYMENT AND RELATED EXPERIENCE

Adjunct Professor 2009-2010
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, T.O. Bonates, V. Kholodovych, P.L. Hammer, R. Langer, D. Anderson, J. Kohn
Logical Analysis of Data in Structure-Property Investigation of Polymeric Gene Delivery. *Macromolecular Theory and Simulations*, 2011, DOI: 10.1002/mats.201000087.
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. *Journal of Chemical Education*, 2010, **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**, 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
^{252}Cf 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 Polymorphyc 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 Academii 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 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.

Manuscripts in progress

A.V. 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