

Yale University Department of Chemistry
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Anastassia N. Alexandrova

Personal

Citizenship: Naturalized citizen of the United States

Education and Training

- 2008-2010 **Postdoctoral.** American Cancer Society Fellow, Theoretical Biophysics. Department of Chemistry, Yale University (under Dr. John Tully)
- 2005-2008 **Postdoctoral.** Computational Biochemistry. Department of Chemistry, Yale University (under Dr. William L. Jorgensen)
- 2005 **Ph.D.** Theoretical Physical Chemistry. Department of Chemistry and Biochemistry, Utah State University. Thesis: "Multiply aromatic clusters via ab initio genetic algorithm" (Advisor Dr. Alexander I. Boldyrev)
- 2000-2001 **Predocctoral.** Computational Analytical Chemistry. Vernadskii Institute of the Russian Academy of Sciences, Moscow, Russia (Advisor Dr. Lev A. Gribov)
- 2000 **M.S.** Chemistry with a specialization in Analytical Chemistry. Honor Diploma. Department of Chemistry, Saratov University, Russia. Thesis: "Sorbition of phenol on synthetic fibrous sorbents" (M.S. Advisor Dr. Lidiya M. Kozlova)
- 1998 **B.S.** Chemistry. Department of Chemistry, Saratov University, Saratov, Russia

Awards and Honors

- 2008-2009 Mary Fieser Postdoctoral Fellowship at Harvard (under Dr. Roy Gordon), \$36K (*declined*)
- 2008-2010 American Cancer Society Postdoctoral Fellowship at Yale (under Dr. John Tully), \$94K
- 2008 Travel Award, National ACS Meeting, Philadelphia, PA
- 2005 Utah State University Robins Award: Graduate Research Assistant of the Year
- 2005 The Utah State University College of Science Graduate Researcher of the Year
- 2005 The Excellence Award of the Chemical Computing Group of the American Chemical Society, National ACS Meeting, San Diego, CA
- 2004-2005 USU School of Graduate Studies Dissertation Fellowship, \$5K
- 2004-2005 Claude E. ZoBell Scholarship for the superior ability to encourage further scientific

- pursuits at Utah State University, College of Science, Utah State University, \$1K
- 2004 Recognition from the American Chemical Society for an Extraordinary Contribution to the Success of the 59th Northwest / 18th Rocky Mountain Regional ACS Meeting
- 2004 Poster Award, 59th Northwest / 18th Rocky Mountain Regional ACS Meeting
- 2004-2005 The one-year sponsored membership in AAAS/Science, the AAAS/Science Program for Excellence in Science
- 2004 Summer Research Institute Fellowship in Interfacial and Condensed Phase Chemical Physics, Pacific Northwest National Laboratory, U.S. Department of Energy, \$1.5K
- 2003-2004 National Deans' List
- 2003 The Chemistry and Biochemistry Alumni Research Award, Utah State University
- 2000 B.S./M.S. Honor Diploma
- 2000 Winner of the Russian Regional Student Olympiad in Chemistry
- 1997-1999 The Scholarship of the Government of Russian Federation for outstanding scientific and academic achievements

Research Experience

2008 - **American Cancer Society Postdoctoral Fellow**

present *Department of Chemistry, Yale University*

Theory of photo-induced processes related to skin cancer.

Constrained DFT methodology for long range charge transfer excited states.

In collaboration with Professor Elsa Yan, Yale University: re-design of binding pockets of proteins for binding unnatural substrates.

In collaboration with Professor Mark Johnson, Yale University: novel gas phase clusters, interpretation of IR-spectra.

2005-2008 **Postdoctoral Associate**

Department of Chemistry, Yale University

In collaboration with Professor Baker, University of Washington: design of artificial enzymes

Mechanisms of enzymatic catalysis. Metallo- β -lactamases. Acyl-CoA carboxylase.

Mechanisms of organic reactions in solution

Development of polarizable force fields

QM/MM Monte Carlo. Free Energy Perturbation method

Visiting Researcher

Sep 2007 *Department of Biochemistry, University of Washington, Laboratory of Professor David Baker (collaboration)*

Enzyme design. Exploring the code of Rosetta package.

July 2004 **Research Fellow**

Environmental Molecular Sciences Laboratory, PNNL

Adaptation of the Genetic Algorithm code for the highly-parallel supercomputer
Boron clusters as potential compounds for the storage of hydrogen

2001-2005 **Graduate Student Researcher**

Department of Chemistry and Biochemistry, Utah State University

Development of the general theory of chemical bonding

Introduction of the multiple aromaticity concept to the inorganic chemistry of main group elements: clusters of boron, lithium, magnesium, and copper; boranes; new classes of aromatic compounds.

In collaboration with Professor Lai-Sheng Wang, PNNL: Interpretation of photoelectron spectra of novel cluster species

Design of new aromatic and antiaromatic inorganic ligands and building blocks

Development and coding of the ab initio Gradient Embedded Genetic Algorithm (GEGA) program searching for global minima of clusters

2000-2001 **Visiting Researcher**

Vernadskii Institute of the Russian Academy of Sciences, Moscow, Russia

Development of a joint computational and IR-spectroscopic method of analysis of chemical wastes

1997-2000 **Undergraduate Research Assistant. Master Student Researcher**

Laboratory of Analytical Chemistry, Department of Chemistry, Saratov University, Russia

Sorption processes for purification of natural waters

Detection of the nitrite-ion in meat products

Undergraduate Research Assistant

1997-1998 *Laboratory of Heterocyclic Compounds, Department of Chemistry, Saratov University, Russia*

Synthesis of compounds with properties of antioxidants

Research Interests

Design of new materials

Artificial enzymes, development of related methods and algorithms

Chemistry of surfaces, defects, and surface-deposited clusters

Hydrogen-storage materials

General theory of chemical bonding, wave-function design

Charge-transfer processes in biology, DNA damage and repair

Stochastic methods. Genetic Algorithms. Algorithm-development.

Alternative interpretations of quantum mechanics

Teaching and Mentoring

2008 Mentoring a Ph.D. student at the Department of Chemistry, Yale University. QM/MM Monte Carlo and Free Energy Perturbation methodology for enzymatic reactions.

2008 Moderating and maintaining the section "Life" on the educational portal, Atomic Scale Design Network" (<http://asdn.net>). Development of the "Enzyme design" section in ASDN. In collaboration with Dr. Anatoli Korkin (Arizona State University).

2008 Yale University series of workshops entitled "Advanced Topics in Science Teaching"

2007 Online mentoring a Master Student at the Department of Chemistry, Saratov University,

- Russia. QM/MM simulations of protein/carbohydrate complexes.
- 2006-2007 Leading a series of informal lectures on Quantum Chemistry for graduate students and postdocs, Yale University.
- 2006 Mentoring a rotation graduate student, Yale University, project on developing a polarized force field method.
- 2005 Yale University 8 weeks course entitled "Mentoring Undergraduate Research"
- 2005 Mentoring a Computer Science M.S. Student programming a Monte Carlo code for the search for the global minima of clusters, Department of Chemistry, Utah State University.
- 2004 Mentoring a Computer Science Undergraduate Student: out joint project of boron hydrides resulted in a co-authored publication. Department of Chemistry, Utah State University.
- 2003 General Chemistry 1230 Laboratory, Utah State University
- 2002 General Chemistry 1210 Laboratory, Utah State University
- 2001 Utah State University Teaching Assistant Workshop
- 2001 Molecular Spectroscopy, lecturing. Department of Chemistry, Saratov University, Russia.
- 2000 Passed the Russian Federation State Exam on Pedagogy, acquired a profession of a pedagogue.
- 1999 Teaching Chemistry in High School (3 classes a week for 2 months), Saratov, Russia.
- 1998-1999 Courses on pedagogy and teaching chemistry, Pedagogy Institute, Saratov, Russia:
- Psychology and pedagogy
 - Interactions of an individual and a group
 - Diagnostics of knowledge, skills, and capabilities of students
 - Methods of teaching chemistry

Teaching Interests

Quantum Mechanics
 Quantum Chemistry (introductory and advanced)
 Physical Chemistry (various sub-areas; undergraduate and graduate levels)
 Molecular Spectroscopy (molecular and electronic structure prospective)
 Computational Chemistry
 Statistical Mechanics
 Biophysical Chemistry / Biophysics
 Material and Surface Chemistry
 General Chemistry (lectures and laboratories).
 Introductory Analytical Chemistry

Course development:

General Chemistry for non-majors
 General Chemistry for students majoring in chemistry.
 Theory of Chemical Bonding and Molecular Design

Professional Services

Affiliations:

American Chemical Society
 Biophysics Society
 New York Academy of Science

American Cancer Society
National Postdoctoral Association

Reviewing manuscripts:

Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Physical Chemistry
Proteins: Structure, Function, and Bioinformatics
Computing in Science & Engineering Magazine
Journal of the American Chemical Society

Conducting scientific meetings:

Reviewing articles for the 12th World Multi-Conference on Systemics, Cybernetics and Informatics: WMSCI 2008, and the 14th International Conference on Information Systems Analysis and Synthesis: ISAS 2008.

Abstract management and web-design for the Regional ACS Meeting of the Northwest / Rocky Mountains Sections, 2004.

Publications

Total citation index: 405, as of Oct 2008 (Web of Knowledge)

1. Journal Articles:

27. Anastassia N. Alexandrova, John C. Tully, Photochemistry of DNA Fragments via Semiclassical Nonadiabatic Dynamics, **2009**, in preparation.

26. Anastassia N. Alexandrova, Daniela Roethlisberger, David Baker, William L. Jorgesen, Balancing the Two Catalytic Modes in Artificial Kemp Elimination Enzymes, **2009**, in preparation.

25. Anastassia N. Alexandrova, Alexander I. Boldyrev, Xiang Li, Harry W. Sarkas, Jay H. Hendricks, Susan T. Arnold, Kit H. Bowen, Lithium Cluster Anions: Photoelectron Spectroscopy and *Ab Initio* Calculations, **2009**, in preparation.

24. Anastassia N. Alexandrova, William L. Jorgensen, The Triple Catalytic Power of the Active Site of the CcrA Metallo- β -Lactamase, **2009**, in preparation.

23. Anastassia N. Alexandrova, William L. Jorgensen, On the Mechanism and Rate of Spontaneous Decomposition of Amino Acids, *J. Am. Chem. Soc.*, **2009**, submitted.

22. Joseph C. Bopp, Anastassia N. Alexandrova, Ben M. Elliott, Tobias Herden, Mark A. Johnson, Infrared vibrational spectra of O_n^- $n = 3-10, 12$ clusters: Isomer evolution of the "core ion" complex, *Int. J. Mass Spec.*, **2009**, 283, 94-99, Professor Bowers 70th birthday special issue.

21. Anastassia N. Alexandrova, William L. Jorgensen, Origin of the Activity Drop with the E50D Variant of Catalytic Antibody 34E4 for Kemp Elimination, *J. Phys. Chem. B* **2009**, 113, 497-504.

20. Anastassia N. Alexandrova, Daniela Roethlisberger, David Baker, William L. Jorgesen, Catalytic Mechanism and Performance of Computationally Designed Enzymes

for Kemp Elimination, *J. Am. Chem. Soc.*, 130, 15907-15915, **2008**.

19. William L. Jorgensen, Kasper P. Jensen, Anastassia N. Alexandrova, Polarization Effects for Hydrogen-Bonded Complexes of Substituted Phenols with Water *J. Chem. Theor. Comput.*, 3, 1987-1992, **2007**.

18. Anastassia N. Alexandrova, William L. Jorgensen, Why Urea Eliminates Ammonia Rather Than Hydrolyzes in Aqueous Solution, *J. Phys. Chem. B* 111, 720-730, **2007**.

17. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua-Jin Zhai, Lai-Sheng Wang, All-Boron Aromatic Clusters as Potential New Inorganic Ligands and Building Blocks in Chemistry, *Coord. Chem. Rev.*, 250, 2811, **2006**.

16. Dmitry Yu. Zubarev, Anastassia N. Alexandrova, Alexander I. Boldyrev, Li-Feng Cui, Xi Li, Lai-Sheng Wang, Alteration of Si_6^{2-} Structure upon Na^+ Coordination in NaSi_6^- , *J. Chem. Phys.*, 124, 124305, **2006**.

15. Anastassia N. Alexandrova, Eldon Koyle, Alexander I. Boldyrev, Theoretical Study of Hydrogenation of Doubly-Aromatic B_7^- , *J. Mol. Model.*, DOI: 10.1007/s00894-005-0035-5, **2005**.

14. Anastassia N. Alexandrova, Alexander I. Boldyrev, Search for the $\text{Li}_x^{0/+1/-1}$ Lowest Energy Structures Using Ab Initio Gradient Embedded Genetic Algorithm (GEGA). Elucidation of the Chemical Bonding in the Lithium Clusters, *J. Chem. Theory Comput.*, 1, 566, **2005**.

13. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua-Jin Zhai, Lai-Sheng Wang, Doubly-Antiaromatic All-Boron Ligand B_6^{2-} in the LiB_6^- molecule. *Ab Initio* and Photoelectron Spectroscopic Study, *J. Chem. Phys.*, 122, 054313, **2005**.

12. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua-Jin Zhai, Lai-Sheng Wang, Cu_3C_4^- – a New Sandwich Molecule with Two Revolving C_2^{2-} Units, *J. Phys. Chem. A*, 109, 562, **2005 (Featured on the Cover)**.

11. Anastassia N. Alexandrova, Alexander I. Boldyrev, You-Jun Fu, Xin Yang, Xue-Bin Wang, Lai-Sheng Wang, Structure of the $\text{Na}_x\text{Cl}_{x+1}^-$ ($x=1-4$) Clusters via *Ab Initio* Genetic Algorithm and Photoelectron Spectroscopy, *J. Chem. Phys.*, 121, 5709, **2004**.

10. Anastassia N. Alexandrova, Hua-Jin Zhai, Lai-Sheng Wang, Alexander I. Boldyrev, Molecular Wheel B_8^{2-} as a New Inorganic Ligand: Photoelectron Spectroscopy and *Ab Initio* Characterization of the LiB_8^- Anion, *Inorg. Chem.*, 43, 3552, **2004**.

9. Anastassia N. Alexandrova, Alexander I. Boldyrev, *Arachno*-, *Nido*- and *Closo*-Aromatic Isomers of the $\text{Li}_6\text{B}_6\text{H}_6$ Molecule, *Inorg. Chem.*, 43, 3588, **2004**.

8. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua-Jin Zhai, Lai-Sheng Wang, Electronic Structure, Isomerism, and Chemical Bonding in B_7^- and B_7 , *J. Phys. Chem. A*, 108, 3509, **2004**.

7. Hua-Jin Zhai, Anastassia N. Alexandrova, Lai-Sheng Wang, Alexander I. Boldyrev, Hepta- and Octacoordinate Boron in Molecular Wheels of Eight- and Nine-Atom Boron

Clusters: Observation and Confirmation, *Angew. Chem. Int. Ed.*, 42, 6004, **2003**.

6. Hua-Jin Zhai, Lai-Sheng Wang, Anastassia N. Alexandrova, Alexander I. Boldyrev, Photoelectron Spectroscopy and *Ab Initio* Study of B_3^- and B_4^- Anions and Their Neutrals, *J. Phys. Chem. A*, 107, 9319, **2003**.

5. Anastassia N. Alexandrova, K. Alexander Birch, Alexander I. Boldyrev, Flattening the $B_6H_6^{2-}$ Octahedron. *Ab Initio* Prediction of the New Family of Planar All-Boron Aromatic Molecules, *J. Am. Chem. Soc. Communications*, 125, 10786, **2003**.

4. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua-Jin Zhai, Lai-Sheng Wang, Erich Steiner, Patrick W. Fowler, Structure and Bonding in B_6^- and B_6 : Planarity and Antiaromaticity, *J. Phys. Chem. A*, 107, 1359, **2003**.

3. Ben Elliott, Anastassia N. Alexandrova and Alexander I. Boldyrev, Hydrogen Trioxide Anion: A Possible Atmospheric Intermediate and Path of Oxygen-Rich Molecules, *J. Phys. Chem. A*, 107, 1203, **2003**.

2. Anastassia N. Alexandrova, Alexander I. Boldyrev, σ -Aromaticity and σ -Antiaromaticity in Alkaline Metal and Alkaline Earth Metal Small Clusters, *J. Phys. Chem. A*, 107, 554, **2003**.

1. Hau-Jin Zhai, Lai-Sheng Wang, Anastassia N. Alexandrova, Alexander I. Boldyrev, Electronic Structure and Chemical Bonding of B_5^- and B_5 by Photoelectron Spectroscopy and *Ab Initio* Calculations, *J. Chem. Phys.*, 117, 7917, **2002**.

2. Published Conference Abstracts:

13. Anastassia N. Alexandrova, William L. Jorgensen, Catalytic mechanism and performance of artificial Kemp elimination enzymes. 236th National ACS Meeting, Philadelphia, PA, August **2008**.

12. Anastassia N. Alexandrova, William L. Jorgensen, David Baker, Artificial enzymes: *in silico* design and QM/MM characterization, book of abstracts, 234th National ACS Meeting, Boston, MA, August **2007**.

11. Anastassia N. Alexandrova, William L. Jorgensen, The Triple Catalytic Power of the Active Site of the CcrA Metallo- β -Lactamase, Electronic Computational Chemistry Conference, April, **2007**.

10. Anastassia N. Alexandrova, William L. Jorgensen, Hydrolysis of β -lactam via *Ab Initio* and QM/MM Simulations, book of abstracts, 232rd National ACS Meeting, San Francisco, CA, September **2006**.

9. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua Jin Zhai, Lai-Sheng Wang, *Ab Initio* Genetic Algorithm Based Elucidation of Multiply Aromatic Clusters, book of abstracts, 229th National ACS Meeting, San Diego, CA, March **2005**.

8. Ben Elliott, Alexander I. Boldyrev, Anastassia N. Alexandrova, Hua Jin Zhai, Xin Yang, Xue Bin Wang, Lai-Sheng Wang, Oxygen Rich Species: Areas of Growth and Advancement, book of abstracts, 229th National ACS Meeting, San Diego, CA, March **2005**.

7. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua-Jin Zhai, Lai-Sheng, Wang, Multiply Aromatic Clusters Via *Ab Initio* Genetic Algorithm, Winter School in Theoretical Chemistry, Helsinki, Finland, December **2004**.
6. Anastassia N. Alexandrova, Alexander I. Boldyrev, The Genetic Algorithm Based Elucidation of the Structure of the Multiply-Aromatic Clusters of Main Group Elements, book of abstracts, 85th Meeting of the AAAS Pacific Division, Logan, UT, June **2004**.
5. Anastassia N. Alexandrova, Alexander I. Boldyrev, The Genetic Algorithm Based Elucidation of the Structure of the σ -Aromatic and σ -Antiaromatic Clusters of Main Group Elements, book of abstracts, 59th Joint Regional Meeting of the Northwest and Rocky Mountain Sections of the ACS, Logan, UT, June **2004**.
4. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hau-Jin Zhai, Lai-Sheng Wang, σ -Aromaticity and σ -Antiaromaticity in Small Clusters of Boron, Lithium and Magnesium, book of abstracts, 227th National ACS Meeting, Anaheim, CA, March **2004**.
3. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hau-Jin Zhai, Lai-Sheng Wang, Multiply Aromatic Small Boron Clusters as New Inorganic Ligands, book of abstracts, 20th Symposium on Molecular Structure, Austin, TX, March **2004**.
2. Ben Elliott, Anastassia N. Alexandrova, Alexander I. Boldyrev, Hau-Jin Zhai, Xin Yang, Xue-Bin Wang, Lai-Sheng Wang, Designing Oxygen-Rich Species: Combining *ab initio* Calculations and Experiment, book of abstracts, 20th Symposium on Molecular Structure, Austin, TX, March **2004**.
1. Anastassia N. Alexandrova, Alexander I. Boldyrev, Hau-Jin Zhai, Lai-Sheng Wang, Aromaticity and Antiaromaticity in Small Boron Clusters and Related Compounds, book of abstracts, 225th National ACS Meeting, New Orleans, LA, USA. March **2003**.

Presentations at Professional Meetings

26. (Oral, invited) Anastassia N. Alexandrova, William L. Jorgensen, Artificial Kemp elimination enzymes: balancing the two catalytic modes, Protein Design Processes, Seattle, WA, September **2008**.
25. (Oral) Anastassia N. Alexandrova, William L. Jorgensen, Catalytic mechanism and performance of artificial Kemp elimination enzymes. 236th National ACS Meeting, Philadelphia, PA, August **2008**.
24. (Poster) Anastassia N. Alexandrova, William L. Jorgensen, Artificial Kemp elimination enzymes: catalytic mechanism and performance via QM/MM Monte Carlo, American Conference on Theoretical Chemistry, Northwestern University, Evanston, IL, July **2008**.
23. (Oral, invited) Anastassia N. Alexandrova, William L. Jorgensen, Artificial Kemp Elimination Enzymes and Retro-Aldolases: QM/MM Monte Carlo Works, Protein Design Processes, Islamorada, FL, December **2007**.
22. (Poster, Invited) Anastassia N. Alexandrova, William L. Jorgensen, Artificial Kemp Elimination Enzymes and Retro-Aldolases: Evaluation and Optimization of the Catalytic

Performance, Protein Design Processes, Islamorada, FL, December **2007**.

21. (Poster, invited) Anastassia N. Alexandrova, William L. Jorgensen, David Baker, Artificial enzymes: *in silico* design and QM/MM characterization. BSM Symposium, Yale University, August **2007**.

20. (Poster) Anastassia N. Alexandrova, William L. Jorgensen, David Baker, Artificial enzymes: *in silico* design and QM/MM characterization. 234th National ACS Meeting, Boston, MA, August **2007**.

19. (Oral, invited) Anastassia N. Alexandrova, William L. Jorgensen, QM/MM Evaluation of Kemp Elimination Theo-zymes, Protein Design Processes, Santa Fe, NM, June **2007**.

18. (Oral, invited) Anastassia N. Alexandrova, William L. Jorgensen, David Baker, Kemp Elimination Theo-zymes, Northeastern Section YCC ACS Chemistry Research Conference, Boston, MA, April **2007**.

17. (Online, invited) Anastassia N. Alexandrova, William L. Jorgensen, The Triple Catalytic Power of the Active Site of the CcrA Metallo- β -Lactamase, Electronic Computational Chemistry Conference, April, **2007**.

16. (Oral, invited) Anastassia N. Alexandrova, William L. Jorgensen, QM/MM Evaluation of Kemp Elimination Theo-zymes, Protein Design Processes, Los Angeles, CA, January **2007**.

15. (Poster) Anastassia N. Alexandrova, William L. Jorgensen, Academic Employment Initiative, 232rd National ACS Meeting, San Francisco, CA, September **2006**.

14. (Poster) Anastassia N. Alexandrova, William L. Jorgensen, Hydrolysis of β -lactam via *Ab Initio* and QM/MM Simulations, 232rd National ACS Meeting, San Francisco, CA, September **2006**.

13. (Oral, invited) Anastassia N. Alexandrova, Ivan Tubert-Brohman, Cristiano Guimarães, William L. Jorgensen, QM/MM/MC Evaluation of Theo-Zyme Performance, Protein Design Processes, Islamorada, FL, April **2006**.

12. (Poster, invited) Anastassia N. Alexandrova, Ivan Tubert-Brohman, Cristiano Guimarães, William L. Jorgensen, QM/MM/MC Simulations of Artificially Designed Aldolases, Protein Design Processes, Islamorada, FL, April **2006**.

11. (Poster) Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua Jin Zhai, Lai-Sheng Wang, *Ab Initio* Genetic Algorithm Based Elucidation of Multiply Aromatic Clusters, 229th National ACS Meeting, San Diego, CA, March **2005**.

10. (Poster) Ben Elliott, Alexander I. Boldyrev, Anastassia N. Alexandrova, Hua Jin Zhai, Xin Yang, Xue Bin Wang, Lai-Sheng Wang, Oxygen Rich Species: Areas of Growth and Advancement, 229th National ACS Meeting, San Diego, CA, March **2005**.

9. (Poster) Anastassia N. Alexandrova, Alexander I. Boldyrev, Hua-Jin Zhai, Lai-Sheng Wang, Multiply Aromatic Clusters Via *Ab Initio* Genetic Algorithm, Winter School in Theoretical Chemistry, Helsinki, Finland, December **2004**.

8. (Poster) Anastassia N. Alexandrova, Alexander I. Boldyrev, The Genetic Algorithm Based Elucidation of the Structure of the Multiply-Aromatic Clusters of Main Group Elements, 85th Meeting of the AAAS Pacific Division, Logan, UT, June **2004**.
7. (Poster) Anastassia N. Alexandrova, Alexander I. Boldyrev, The Genetic Algorithm Based Elucidation of the Structure of the σ -Aromatic and σ -Antiaromatic Clusters of Main Group Elements, 59th Joint Regional Meeting of the Northwest and Rocky Mountain Sections of the ACS, Logan, UT, June **2004**.
6. (Poster) Anastassia N. Alexandrova, Alexander I. Boldyrev, Hau-Jin Zhai, Lai-Sheng Wang, σ -Aromaticity and σ -Antiaromaticity in Small Clusters of Boron, Lithium and Magnesium, 227th National ACS Meeting, Anaheim, CA, March **2004**.
5. (Poster) Anastassia N. Alexandrova, Alexander I. Boldyrev, Hau-Jin Zhai, Lai-Sheng Wang, Multiply Aromatic Small Boron Clusters as New Inorganic Ligands, 20th Symposium on Molecular Structure, Austin, TX, March **2004**.
4. (Poster) Ben Elliott, Anastassia N. Alexandrova, Alexander I. Boldyrev, Hau-Jin Zhai, Xin Yang, Xue-Bin Wang, Lai-Sheng Wang, Designing Oxygen-Rich Species: Combining *ab initio* Calculations and Experiment, 20th Symposium on Molecular Structure, Austin, TX, March **2004**.
3. (Poster) Anastassia N. Alexandrova, Alexander I. Boldyrev, Hau-Jin Zhai, Lai-Sheng Wang, Aromaticity and Antiaromaticity in Small Boron Clusters and Related Compounds, 225th National ACS Meeting, New Orleans, LA, USA. March **2003**.
2. (Oral) Anastassia N. Alexandrova, Lidia M. Kozlova, Sorbtion of Phenol on Synthetic Fibrous Sorbents, B.S./M.S. Diploma Public Defense, June, **2000**.
1. (Oral) Anastassia N. Alexandrova, Rimma K. Chernova, Analytical Detection of the Nitrite Ion in Meat Products, Undergraduate Student Conference, Saratov, Russia, May, **1998**.

Invited Talks

- 2009 University of Notre Dame, Department of Chemistry
University of Colorado, Boulder, Department of Chemistry and Biochemistry
Syracuse University, Department of Chemistry
University of Virginia, Department of Chemistry
University of California, Los Angeles, Department of Chemistry and Biochemistry
- 2008 University of California, Merced, School of Natural Sciences
Brown University, Department of Chemistry
University of the Virgin Inlands, School of Mathematics and Science
University of Maryland at College Park, Energy Research Center, College of Engineering
Colorado School of Mines, Department of Chemistry and Geochemistry
University of Georgia, Department of Chemistry
Massachusetts Institute of Technology, Department of Chemical Engineering
Johns Hopkins University, School of Medicine, Department of Biophysics and Biophysical Chemistry
Stanford University, Department of Chemical Engineering
- 2007 University of Washington, Department of Chemistry

University of Vermont, Department of Chemistry
University of California, Berkeley, Department of Chemical Engineering
Worcester Polytechnic Institute, Department of Chemistry

2006 Michigan Technological University, Department of Chemistry
Illinois Institute of Technology, Department of Chemical and Environmental Engineering
San Francisco State University, Department of Chemistry
Wichita State University, Department of Chemistry

Collaborators

Kit Bowen (Johns Hopkins University)
David Baker (University of Washington)
Daniela Roethlisberger (University of Washington)
Mark Johnson (Yale University)
Joseph Bopp (Yale University)
Ben Elliott (Yale University)
Elsa Yan (Yale University)
Lai-Sheng Wang (Pacific Northwest National Laboratory)
Hua-Jin Zhai (Pacific Northwest National Laboratory and Washington State University)
You-Jun Fu (Pacific Northwest National Laboratory and Washington State University)
Xin Yang (Pacific Northwest National Laboratory and Washington State University)
Xue-Bin Wang (Pacific Northwest National Laboratory and Washington State University)
Patrick Fowler (University of Sheffield, UK)
Eric Steiner (University of Exeter, UK)
Nikolay Dokholyan (University of North Carolina at Chapel Hill)
Anatoli Korkin (Arizona State University)
Dmitry Zubarev (UC Berkeley)

Professional References

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Steve Scheiner, Professor and Department Head

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