

Dr. Alexander S. Ivanov

Curriculum Vitae

Chemical Sciences Division
Oak Ridge National Laboratory
Oak Ridge TN, 37831 USA
Office A105

E-mail: ivanova@ornl.gov

Website: <https://ornl.gov/staff-profile/aleksandr-ivanov>

Phone: +1 (865) 576-1753

Personal data

Born on 02.26.1988 in Tula, Russia
Languages: English (fluent), Russian (native)

Academic Degrees

- Ph. D.** Theoretical Physical Chemistry. *Aug 2011 – Aug 2015*
Department of Chemistry and Biochemistry, Utah State University
Graduate Advisor: Dr. Alex I. Boldyrev
- M. Sc.** Physical Chemistry. *Summa cum laude.* *Sept 2010 – June 2012*
Department of Science, PFUR, Moscow
Graduate Advisor: Dr. Konstantin V. Bogenko
- B. Sc.** Chemistry. *Summa cum laude.* *Sept 2005 – June 2010*
Department of Science, PFUR, Moscow
Undergraduate Advisor: Dr. Konstantin V. Bogenko

Awards and Honors

- Marjorie H. Gardner Teaching Award**, Utah State University *2015*
- Outstanding Graduate Student in Chemistry Award**, Utah State University *2014*
- Award for Early Research Progress in Chemistry**, Utah State University *2013*
- USU Graduate Division Research Travel Grant**, Utah State University *2013*
- M. Sc. Honor Diploma (*Summa cum laude*)**, PFUR, Moscow *2012*
- Dr. Gryaznov Memorial Award for Excellence in Science**, PFUR, Moscow *2010*
- Best Graduate Student in Science – 2010 Award**, PFUR, Moscow *2010*
- B. Sc. Honor Diploma (*Summa cum laude*)**, PFUR, Moscow *2010*
- Russian Government Scholarship for Outstanding Academic Achievements** *2005 – 2012*

Research Experience

Oak Ridge National Laboratory, Tennessee USA
Postdoctoral Research Associate

2015 – present

Utah State University, Utah USA
Doctoral Research – advisor: Dr. Alex I. Boldyrev

2011 – 2015

- Applied novel computational methods with the aim of predicting and understanding the behavior of new molecules, clusters, and materials, including fundamentally interesting and technologically useful inorganic double helical nanostructures.
- Investigated electronic and structural characteristics of clusters and their size-dependent properties using *ab initio* quantum chemistry calculations.
- Performed chemical bonding analyses in organometallic complexes, porphyrins, solid state materials, and clusters using Adaptive Natural Density Partitioning and other state-of-the-art methods.
- Studied effects of microsolvation on the stability of dichloride anion pair to understand complicated processes of solvation of Cl^- in the condensed phases.
- Wrote a program for theoretical simulation of Frank-Condon vibrational progression to interpret and analyze experimental photoelectron spectra results.

PFUR, Moscow Russia
Graduate Research – advisor: Dr. Konstantin V. Bogenko

2010 – 2011

- Performed quantum chemical studies of mixed boron-carbon anion species.

PFUR, Moscow Russia
Undergraduate Research – advisor: Dr. Konstantin V. Bogenko

2008 – 2010

- Investigated chemical bonding in boron clusters.

PFUR, Moscow Russia
Undergraduate Research – advisor: Dr. Tatiana N. Borisova

2006 – 2008

- Performed organic synthesis and investigated the reactionary capability of nitrogen-bearing heterocyclic species and biologically active compounds.

Teaching Experience

CHEM 1225. Principles of Chemistry II. Utah State University

Spring 2015

CHEM 2325. Organic Chemistry II. Utah State University

Spring 2014

CHEM 1215. Principles of Chemistry I. Utah State University	<i>Spring 2013</i>
CHEM 1215. Principles of Chemistry I. Utah State University	<i>Spring 2012</i>
College Level Chemistry Teaching. PFUR, Moscow 1 semester course and practical training	<i>Fall 2010</i>

Skills and Activities

<i>Skills:</i>	Programming: C/C++, Python Experienced user of quantum chemistry packages such as Gaussian, Molpro, and The Vienna Ab-initio Simulation Package (VASP) Operating Systems: Unix/Linux, Mac, Windows
<i>Research Interests:</i>	Computational chemistry, quantum mechanics, electronic structure theory, energy and chemical processes, catalysis, chemical separation, materials design
<i>Internships:</i>	Agilent Technologies, Inc., Russian Office (Moscow). Summer 2010
<i>Memberships:</i>	American Chemical Society (ACS) since 2011
<i>Reviewer for:</i>	Journal of the American Chemical Society (ACS Publications), Journal of Chemical Theory and Computation (ACS Publications), Journal of Chemical Physics (AIP) Molecular Physics

Conference Proceedings and Seminars

<i>03/2015</i>	249 th National ACS Meeting & Exposition. Division of Physical Chem. “ <i>Stabilization of a Cl⁻Cl⁻ Anion Pair in the Gas Phase: Ab initio Microsolvation Study</i> ”, Denver, CO, USA; (Poster)
<i>10/2014</i>	19 th International Conference on Commercializing Micro- and Nanotechnology. “ <i>Inorganic Double-Helix Nanocoils for Future Microelectronic Devices</i> ”, Salt Lake City, UT, USA; (Poster)
<i>09/2014</i>	Chemistry and Biochemistry Departmental Seminar, “ <i>Reliable Predictions of New Molecules, Clusters, and Materials Using Computational Methods</i> ”, Logan, UT, USA; (Talk)
<i>07/2014</i>	2 nd International Conference on Chemical Bonding, Kauai, HI, USA (administrative support)
<i>11/2013</i>	Physical and Analytical Chemistry Seminar, “ <i>Quantum Chemical Studies of Novel LiP Clusters and LiP Nanowires</i> ”, Logan, UT, USA; (Talk)
<i>04/2013</i>	245 th National ACS Meeting & Exposition. Division of Inorganic Chem. “ <i>Simplest inorganic double-helix structures</i> ”, New Orleans, LA, USA; (Poster)

Publications

Sum of the times cited (as of 11/25/2015): **137** (Google Scholar), **108** (ISI Web of Knowledge)
H-index: **8** (Google Scholar), **7** (ISI Web of Knowledge) since 2011

Oak Ridge National Laboratory (2015-present)

- [19] N. Mehio, **A. S. Ivanov**, A. P. Ladshaw, S. Dai, V. Bryantsev, “Theoretical Study of Oxovanadium(IV) Complexation with Formamidoximate: Implications for the Design of Uranyl-Selective Adsorbents” *Ind. Eng. Chem. Res.*, DOI: 10.1021/acs.iecr.5b03398 2015 [impact factor = 2.6]
- [18] R. Custelcean, N. J. Williams, C. A. Seipp, **A. S. Ivanov**, V. Bryantsev, “Aqueous Sulfate Separation by Sequestration of $[(\text{SO}_4)_2(\text{H}_2\text{O})_4]^{4-}$ Clusters within Highly Insoluble Imine-Linked Bis-Guanidinium Crystals” *Chem. Eur. J.*, *accepted*, 2015 [impact factor = 5.7]

Utah State University (2011-2015); * denotes corresponding author

- [17] **A. S. Ivanov**,* T. Kar, A. I. Boldyrev, “Nanoscale Stabilization of Zintl Phase Compounds: 1D Ionic LiP Chain Confined Inside a Carbon Nanotube” 2015. *Under revision*
- [16] A. S. Nizovtsev, **A. S. Ivanov**, A. I. Boldyrev, S. N. Konchenko, “ Li_4E_8 (E = P, As, Sb, Bi) Clusters: The Quest for Realgar-Type $[\text{E}_8]^{4-}$ Zintl Anions” *Eur. J. Inorg. Chem.*, DOI: 10.1002/ejic.201500931, 2015 [impact factor = 2.9]
- [15] **A. S. Ivanov**, X. Zhang, A. I. Boldyrev, K. H. Bowen Jr., I. Černušák, “Anion Photoelectron Spectroscopy and CASSCF/CASPT2/RASSI Study of La_n^- (n = 1, 3-7)” *J. Phys. Chem. A*, 119, 11293-11303, 2015 [impact factor = 2.8]
- [14] J. A. Dolyniuk, H. He, **A. S. Ivanov**, A. I. Boldyrev, S. Bobev, K. Kovnir “Ba and Sr Binary Phosphides: Synthesis, Crystal Structures, and Bonding Analysis” *Inorganic Chemistry*, 54, 8608-8616, 2015 [impact factor = 4.8]
- [13] **A. S. Ivanov**, E. Miller, A. I. Boldyrev, Y. Kameoka, T. Sato, K. Tanaka, “Pseudo Jahn-Teller Origin of Buckling Distortions in Two-Dimensional Triazine-Based Graphitic Carbon Nitride ($\text{g-C}_3\text{N}_4$) Sheets” *J. Phys. Chem. C*, 119, 12008-12015, 2015 [impact factor = 4.8]
- [12] **A. S. Ivanov**, I. A. Popov, A. I. Boldyrev, V. V. Zhdankin, “The I=X (X = O, N, C) Double Bond in Hypervalent Iodine Compounds: Is It Real?” *Angew. Chem. Int. Ed.*, 53, 9617-9621, 2014 [impact factor = 13.7]
Highlighted in Chemistry World, 2014, July 11
- [11] **A. S. Ivanov**, A. I. Boldyrev, “Deciphering Aromaticity in Porphyrinoids via Adaptive Natural Density Partitioning” *Org. Biomol. Chem.*, 12, 6145-6150, 2014 [impact factor = 3.5]

- [10] J. K. Olson, **A. S. Ivanov**, A. I. Boldyrev, "All-Nitrogen Analogue of Ozone: Li_3N_3 Species" *Chem. Eur. J.*, 20, 6636-6640, 2014 [impact factor = 5.7]
- [9] **A. S. Ivanov**, A. I. Boldyrev, G. Frenking, "Inorganic Double-Helix Nanotoroid of Simple Lithium-Phosphorus Species" *Chem. Eur. J.*, 20, 2431-2435, 2014 [impact factor = 5.7]
*Featured on the cover of the **Chemical & Engineering News**, 2014, Vol. 92, Issue 38*
- [8] **A. S. Ivanov**, G. Frenking, A. I. Boldyrev, "Stabilization of Cl^-Cl^- Anion Pair in the Gas Phase: Ab Initio Microsolvation Study" *J. Phys. Chem. A*, 118, 7375-7384, 2014 (K. D. Jordan Festschrift) [impact factor = 2.8]
*Highlighted in **Chemistry Views**, 2014, March 04*
- [7] W. L. Li, **A. S. Ivanov**, J. Federic, C. Romanescu, I. Cernusak, A. I. Boldyrev, L.-S. Wang, "On the way to the highest coordination number in the planar metal-centred aromatic $\text{Ta}@\text{B}_{10}$ cluster: Evolution of the Structures of TaB_n^- ($n = 3-8$)" *J. Chem. Phys.*, 139, 104312, 2013 [impact factor = 3.1]
- [6] **A. S. Ivanov** and A. I. Boldyrev, "Reliable Predictions of Unusual Molecules" *Phys. Chem. Chem. Phys.*, 14, 15943-15952, 2012 (invited review article) [impact factor = 4.2]
*Designated a "Hot Article" by **Phys. Chem. Chem. Phys. Journal**, 2012, November 09*
- [5] **A. S. Ivanov** and A. I. Boldyrev, " $\text{Si}_{6-n}\text{C}_n\text{H}_6$ ($n = 0-6$) Series: When Do Silabenzenes Become Planar and Global Minima?" *J. Phys. Chem. A*, 116, 9591-9598, 2012 [impact factor = 2.8]
- [4] **A. S. Ivanov**, K. V. Bozhenko, A. I. Boldyrev, "On the Suppression Mechanism of the Pseudo-Jahn-Teller Effect in Middle E_6 ($E = \text{P}, \text{As}, \text{Sb}$) Rings of Triple-Decker Sandwich Complexes" *Inorganic Chemistry*, 8, 8868-8872, 2012 [impact factor = 4.8]
- [3] **A. S. Ivanov**, A. J. Morris, K. V. Bozhenko, C. J. Pickard, A. I. Boldyrev, "Inorganic Double-Helix Structures of Unusually Simple Li-P Species" *Angew. Chem. Int. Ed.*, 33, 8330-8333, 2012 [impact factor = 13.7]
Highlighted in:
***Chemical & Engineering News**, 2012, Vol. 90, Issue 33;*
***The London Centre for Theory and Simulation of Materials (UK)**, 2012, August 15;*
***Utah State Today**, 2012, August 16; and other media*
- [2] **A. S. Ivanov**, K. V. Bozhenko, A. I. Boldyrev, "Peculiar Transformations in the $\text{C}_x\text{H}_x\text{P}_{4-x}$ ($x = 0-4$) Series" *J. Chem. Theor. Comput.*, 8, 135-140, 2011 [impact factor = 5.3]
- [1] T. R. Galeev, **A. S. Ivanov**, C. Romanescu, W.-L. Li, K. V. Bozhenko, L.-S. Wang, A. I. Boldyrev, "Molecular Wheel to Monocyclic Ring Transition in Boron-Carbon Mixed Clusters C_2B_6^- - C_3B_5^- " *Phys. Chem. Chem. Phys.*, 13, 8805-8810, 2011 [impact factor = 4.2]

Collaboration

Prof. L.-S. Wang, Brown University (USA)

- Interpreted photoelectron spectra of clusters in the gas phase and performed *ab initio* quantum chemistry calculations to elucidate electronic and structural characteristics of clusters.

Prof. C. J. Pickard, University College London (UK)

- Performed global minimum search of Li_nP_n ($n=5-9$) species and rationalized chemical bonding in LiP double helical nanostructures.

Prof. K. Kovnir, University of California Davis (USA)

- Analyzed chemical bonding in the newly synthesized Zintl phase solid state compounds SrP_2 , BaP_2 , Ba_5P_4 using Solid State Adaptive Natural Density Partitioning approach.

Prof. T. Sato, Kyoto University (Japan)

- Investigated pseudo Jahn-Teller effect in 2D triazine-based graphitic carbon nitride sheets.

E. Emmet Reid Prof. K. H. Bowen, Johns Hopkins University (USA)

- Interpreted photoelectron spectra and chemical bonding of La_n^- ($n=1-3$) clusters.

Prof. (Editor of J. Comput. Chem.) G. Frenking, Philipp University of Marburg (Germany)

- Performed a systematic *ab initio* study of microsolvation of dichloride anion pair in the gas phase; investigated the stability of the first inorganic LiP double helical nanotoroid system.

References

A. I. Boldyrev, Ph. D.

Professor
Department of Chemistry
and Biochemistry,
Utah State University
0300 Old Main Hill
Logan, UT 84322-0300
+1 (435) 7971630
a.i.boldyrev@usu.edu

G. Frenking, Ph. D.

Professor, Editor of JCC
Department of Chemistry,
Philipp University of
Marburg, Germany
Hans-Meerweinstr. 4
Marburg, D35039, Germany
+49 (6421) 2825563
frenking@chemie.uni-marburg.de

L.-S. Wang, Ph. D.

Professor
Department of Chemistry
and Biochemistry,
Brown University, RI
324 Brook Street
Providence, RI 02912
+1 (401) 8633389
Lai-Sheng_Wang@brown.edu