

Dept. of Chemistry and Biochemistry
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Education:

- 2007 - 2012** **Ph.D. in Chemistry** Department of Chemistry and Biochemistry, Utah State University
GPA=4.0 emphasis: physical/theoretical/computational/quantum chemistry
Graduate Advisor: A. I. Boldyrev
- 2002 - 2007** **B.Sc. in Chemistry** Department of Science, Peoples' Friendship University of Russia, Moscow
GPA=4.0 Undergraduate Advisor: K. V. Bogenko

Awards and Honors:

- 2012 **The Marjorie H. Gardner Teaching Award**, USU.
2012 **The 2011-2012 College of Science Ph. D. Graduate Researcher of the Year**, USU.
2011 **American Chemical Society Physical Chemistry Division Outstanding Student Poster Award**
at the 242nd American Chemical Society National Meeting, Denver, CO.
2011 **The School of Graduate Studies Dissertation Fellowship**, USU.
2011 **The Outstanding Graduate Student in Chemistry Award**, USU.
2010 **American Chemical Society Physical Chemistry Division Outstanding Student Poster Award**
at the 239th American Chemical Society National Meeting, San Francisco, CA.
2010 **IBM-Zerner Award for Graduate Students**
at the 50th Sanibel Symposium, Quantum Theory Project, St. Simons Island, GA.
2008 **Award for Early Research Progress in Chemistry**, USU.
2007 **B.Sc. Honor Diploma**, PFUR.

Research Experience:

- 2007 - present** **Graduate Researcher**
Research Group of Alexander I. Boldyrev
Department of Chemistry and Biochemistry
Utah State University, Logan, UT, USA

Development of chemical bonding theory in pure and doped clusters composed of boron, gold, aluminum, transition metals,[†] etc. via introducing multiple aromaticity/antiaromaticity/conflicting aromaticity concepts and performing the newly developed Adaptive Natural Density Partitioning method. Extending the gained experience in chemical bonding from cluster species to solids.

Interpretation of photoelectron spectra of novel clusters that have the potential to be building blocks of future nanomaterials and nanocatalysts.*#

Investigating peculiarities of multiply charged anions: stability, reactivity, phenomenon of negative electron binding energy, mechanisms of solvation, etc.*§

Rationalizing non-stability of high-symmetry structures via Jahn-Teller Effects (Pseudo Jahn-Teller Effect, Renner-Teller Effect).[◇]

Investigating the nature of molecular motors.^{††}

In collaboration with:

* Professor Lai-Sheng Wang, Brown University

Professor Kit H. Bowen, Johns Hopkins University

§ Prof. Manfred M. Kappes and Prof. Oliver Hampe, The Institute of Nanotechnology, Karlsruhe, Germany

◇ Dr. Konstantin Pokhodnya, Center of Nanoscale Science and Engineering, North Dakota State University

† Prof. Philippe F. Weck, University of Nevada Las Vegas

†† Prof. Gabriel Merino, Universidad de Guanajuato, Mexico

†† Prof. Thomas Heine, Jacobs University, Germany

†† Prof. Jesus Ugalde, Donostia International Physics Center, Spain

†† Prof. Anastassia Alexandrova, University of California, Los Angeles

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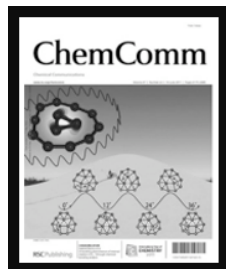
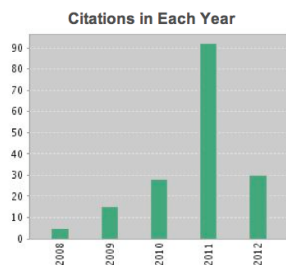
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LIST OF PUBLICATIONS:

20 papers (4 communications + 3 invited chapters + 1 invited article + 12 peer reviewed articles)

Sum of the times cited 170 (as of April 7, 2012)

h-index 7 (as of April 7, 2012)



20. Z. A. Piazza, W.L. Li, C. Romanescu, **A. P. Sergeeva**, L. S. Wang, A. I. Boldyrev. *J. Chem. Phys.* 2012, 136, 104310
19. **A. P. Sergeeva**, B. B. Averkiev, H. J. Zhai, A. I. Boldyrev, L. S. Wang. *J. Chem. Phys.* 2011, 134, 224304
JCP Editors' Choice for 2011
18. **A. P. Sergeeva**, A. I. Boldyrev. *J. Clust. Sci.* 2011, 22, 321-329 (invited article)
17. T. R. Galeev, Q. Chen, J. C. Guo, H. Bai, C. Q. Miao, H. G. Lu, **A. P. Sergeeva**, S. D. Li, A. I. Boldyrev. *Phys. Chem. Chem. Phys.* 2011, 13, 11575-11578 (communication)
16. C. Romanescu, **A. P. Sergeeva**, W. L. Li, A. I. Boldyrev, L. S. Wang. *J. Am. Chem. Soc.* 2011, 133, 8646-8653
15. G. Martinez-Guajardo, **A. P. Sergeeva**, A. I. Boldyrev, T. Heine, J. M. Ugalde, G. Merino. *Chem. Comm.*, 2011, 47, 6242-6244 (communication)
Featured on the cover
14. K. Pokhodnya, C. Olson, X. Dai, D. L. Schulz, P. Boudjouk, **A. P. Sergeeva**, A. I. Boldyrev. *J. Chem. Phys.*, 2011, 134, 014105
13. P. F. Weck, **A. P. Sergeeva**, E. Kim, A. I. Boldyrev, and K. R. Czerwinski. *Inorg. Chem.*, 2011, 50, 1039-1046
12. **A. P. Sergeeva**, A. I. Boldyrev. In *Aromaticity and Metal clusters. Atoms, Molecules, and Clusters. Structure, Reactivity, and Dynamics book series. P. K. Chattaraj, Ed.*; CRC Press, Taylor & Francis Group, Boca Raton, 2010, pp. 55-68. (invited chapter)
11. **A. P. Sergeeva**, A. I. Boldyrev. *Phys. Chem. Chem. Phys.*, 2010, 12, 12050-12054 (communication)
10. **A. P. Sergeeva**, A. I. Boldyrev. *Organometallics*, 2010, 29, 3951-3954
9. H. Wang, Y. J. Ko, K. H. Bowen, **A. P. Sergeeva**, B. B. Averkiev, A. I. Boldyrev. *J. Phys. Chem. A*, 2010, 114, 11070-11077
8. **A. P. Sergeeva**, B. B. Averkiev, A. I. Boldyrev. In *Metal-Metal Bonding. Structure and Bonding book series. G. Parkin, Ed.*; Volume 136, Springer, Berlin/Heidelberg, 2010, pp. 275-306. (invited chapter)
7. **A. P. Sergeeva**, A. I. Boldyrev. *Comm. Inorg. Chem.*, 2010, 31, 2-12
6. W. Huang, **A. P. Sergeeva**, H. J. Zhai, B. B. Averkiev, L. S. Wang, A. I. Boldyrev. *Nature Chemistry*, 2010, 2, 202-206
Highlighted in C&EN, Vol. 88, Issue 28, p. 9 and in Chemistry World, Vol.7, No.3, 2010
5. X. B. Wang, **A. P. Sergeeva**, X. P. Xing, M. Massaouti, T. Karpuschkin, O. Hampe, A. I. Boldyrev, M. Kappes, L. S. Wang. *J. Am. Chem. Soc.*, 2009, 131, 9836-9842
4. X. B. Wang, **A. P. Sergeeva**, J. Yang, X. P. Xing, A. I. Boldyrev, L. S. Wang. *J. Phys. Chem. A*, 2009, 113, 5567-5576
3. D. Yu. Zubarev, **A. P. Sergeeva**, A. I. Boldyrev. In *Chemical Reactivity Theory. A Density Functional View. Chattaraj, P. K., Ed.*; CRC Press. Taylor & Francis Group: New York, 2009, pp. 439-452. (invited chapter)
2. **A. P. Sergeeva**, D. Yu. Zubarev, H. J. Zhai, L. S. Wang, A. I. Boldyrev. *J. Am. Chem. Soc.*, 2008, 130, 7244-7246 (communication)
1. J. Yang, X. P. Xing, X. B. Wang, L. S. Wang, **A. P. Sergeeva**, A. I. Boldyrev. *J. Chem. Phys.*, 2008, 128, 091102

To access the papers go to: ion.chem.usu.edu/~boldyrev/alina

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Presentations at Professional Meetings:

- 08/28 – 09/01, 2011 *"Rationalizing chemical bonding in molecular Wankel motors"*
Division of Physical Chemistry, at the 242nd National ACS Meeting, Denver, CO.
- 03/21 – 03/25, 2010 *"Structure, stability and unique chemical bonding of pure boron clusters: All-boron hydrocarbon analogs"*
Division of Physical Chemistry, at the 239th National ACS Meeting, San Francisco, CA.
- 03/21 – 03/25, 2010 *"Deciphering chemical bonding: From clusters to solids"*
Division of Inorganic Chemistry, at the 239th National ACS Meeting, San Francisco, CA.
- 02/24 – 03/02, 2010 *"Towards unified chemical bonding theory"*
The 50th Sanibel Symposium, Quantum Theory Project, St. Simons Island, GA.
- 06/13, 2009 *"Ab Initio, Photoelectron Spectroscopy, and Mass-Spectroscopic probing of negative electron binding energy, electronic structure and stability of isolated and solvated multiply-charged anions"*
Celebration of 40 Years of Ion chemistry, Carl Lineberger and His Co-Conspirators, Boulder, CO.
- 08/17 – 08/21, 2008 *"Peculiarities of 1-hydroxy-3,6,8-pyrene-trisulfonate triply charged anion"*
Division of Physical Chemistry, at the 236th National ACS Meeting, Philadelphia, PA.

Teaching Experience:

- 2010-2011 Teaching Assistantship, General Chemistry 1210 Recitations, USU, Logan, UT.
- 2010 Process Oriented Guided Inquiry Learning Workshop, Westminster College, Salt Lake City, UT.
- 2007 Teaching Assistant Workshop, Utah State University, Logan, UT.
- 2006 One semester course in pedagogy, PFUR, Moscow, Russia.

Mentoring:

Graduate Students

Timur Galeev (2009-present); Ivan Popov (2009-present); Caleb Allpress (2009); Andrey Vorobiev (2008); Alexander Ivanov (2009-present).

Highschool Students

Philip Cutler (2011); Dustin Hicken (2010); Rebekah Jung (2009); Ellie Edwards (2008) within the Summer Internship Program at USU.

Career objective:

Pursue a scientific career in academia

Professional Activities:

- 2009 – 2011 Departmental Representative of Graduate Student Senate at USU
- 2008 – present Member of American Chemical Society

Professional References:

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