

## LIST OF PUBLICATIONS AND PRESENTATIONS

(June 2008)

Dmitry Yu. Zubarev

1. "Comment on Instability of the  $Al_4^{2-}$  'All-Metal Ion' and Its Implications", Zubarev, D. Yu.; Boldyrev, A. I. (accepted for the publication in *J. Phys. Chem. A*)
2. "Developing Paradigms of Chemical Bonding: Adaptive Natural Density Partitioning", Zubarev, D. Yu.; Boldyrev, A. I. (accepted for the publication in *PCCP*)
3. "Multiple Aromaticity, Multiple Antiaromaticity, and Conflicting Aromaticity in Planar Clusters", Zubarev, D. Yu.; Boldyrev, A. I. (chapter in the book "Clusters - a Bridge Across Disciplines", in press)
4. "Multifold Aromaticity, Multifold Antiaromaticity, and Conflicting Aromaticity. Implications for Stability and Reactivity of Clusters", Zubarev, D. Yu.; Sergeeva, A. P.; Boldyrev, A. I. (chapter in the book "Theory of Chemical Reactivity", in press)
5. "Carbon Avoids Hypercoordination in  $CB_6^-$ ,  $CB_6^{2-}$ , and  $C_2B_5^-$  Planar Carbon-Boron Clusters", Averkiev, B. B.; Zubarev, D. Yu.; Wang, L. M.; Huang, W.; Wang, L. S.; Boldyrev, A. I. *J. Am. Chem. Soc.* Published online (**communication**)
6. "A Photoelectron Spectroscopic and Theoretical Study of  $B_{16}^-$  and  $B_{16}^{2-}$ : An All-Boron Naphthalene", Sergeeva, A. P.; Zubarev, D. Yu.; Zhai, H. -J.; Boldyrev, A. I.; Wang, L. S. *J. Am. Chem. Soc.* published online (**communication**).
7. "Aromaticity and antiaromaticity in transition-metal systems", Zubarev, D. Yu.; Averkiev, B. B.; Zhai, H. -J.; Wang, L. S.; Boldyrev, A. I. *Phys. Chem. Chem. Phys.* **2008**, *10*, 257 (**cover page**)
8. " $\delta$ -Aromaticity in  $Ta_3O_3^-$ : A New Mode of Chemical Bonding", Zhai, H.-J.; Averkiev, B. B.; Zubarev, D. Yu.; Wang, L. S.; Boldyrev, A. I. *Angew. Chem. Int. Ed.* **2007**, *46*, 4277 (**highlighted in Chemical and Engineering News, May 7, 2007, 54**).
9. "On the Chemical Bonding of Gold in Auro-Boron Oxide Clusters  $Au_nBO^-$  ( $n=1-3$ )", Zubarev, D. Yu.; Boldyrev, A. I.; Li, J.; Zhai, H.-J.; Wang, L. S. *J. Phys. Chem. A*, **2007**, *111*, 1648.
10. "Global Minimum Structure Searches via Particle Swarm Optimization", Call, S. T.; Zubarev, D. Yu.; Boldyrev, A. I. *J. Comput. Chem.* **2007**, *28*, 1177.
11. "Comprehensive Analysis of Chemical Bonding in Boron Clusters", Zubarev, D. Yu.; Boldyrev, A. I. *J. Comput. Chem.* **2006**, *28*, 251 (**Special Issue: 90 Years of Chemical Bonding; cover page of vol. 28, iss. 2-5**).
12. " $Sn_{12}^{2-}$ : Stannaspherene", Cui, L. F.; Huang, X.; Wang, L. M.; Zubarev, D. Yu.;

- Boldyrev, A. I.; Li, J.; Wang L. S. *J. Am. Chem. Soc.* **2006**, *128*, 8390 (**communication**).
13. "Theoretical Probing of Deltahedral Closo-Auro-Boranes  $B_xAu_x^{2-}$  ( $x = 5-12$ )", Zubarev, D. Yu.; Li, J.; Wang, L. S.; Boldyrev, A. I. *Inorg. Chem.* **2006**, *45*, 5269 (**communication**).
  14. "Observation of Triatomic Species ( $AlSi_2^-$  and  $AlGe_2^-$ ) With Conflicting Aromaticity", Zubarev, D. Yu.; Boldyrev, A. I.; Li, X.; Wang, L. S. *J. Phys. Chem. B*, **2006**, *110*, 9743 (**communication**).
  15. "On the Structure and Chemical Bonding of  $Si_6^{2-}$  and  $Si_6^{2-}$  in  $NaSi_6^-$  upon  $Na^+$  Coordination." Zubarev, D. Yu.; Alexandrova, A.; Boldyrev, A. I.; Cui, L. F.; Li, X.; Wang, L. S. *J. Chem. Phys.* **2006**, *124*, 124305.
  16. "Gold apes hydrogen. The structure and bonding in the planar  $B_7Au^{2-}$  and  $B_7Au_2$  clusters." Zhai, H.-J.; Wang, L. S.; Zubarev, D. Y.; Boldyrev A. I. *J. Phys. Chem. A*, **2006**, *110*, 1689 (**communication, cover page**).
  17. "Chemical bonding in  $Si_5^{2-}$  and  $NaSi_5^-$  via Photoelectron Spectroscopy and Ab Initio Calculations." Zubarev, D. Yu.; Boldyrev, A. I.; Li, X.; Cui, L. F.; Wang, L. S. *J. Phys. Chem. A* **2005**, *109*, 11385.
  18. "Appraisal of the performance of nonhybrid density functional methods in characterization of the  $Al_4C$  molecule." Zubarev, D. Yu.; Boldyrev, A. I. *J. Chem. Phys.* **2005**, *122*, 144322.

## PRESENTATIONS

1. "Analysis of chemical bonding in clusters by means of the adaptive natural density partitioning", PhD defense, Department of Chemistry and Biochemistry, Utah State University, March 24, 2008.
2. "Evolution of the paradigms of chemical bonding", oral presentation, 22nd Austin Symposium on Molecular Structure, Austin, TX, March 1-4, 2008.
3. "Breakdown of the spherical symmetry in semiconducting sub-nanoclusters", talk at the Club Med seminar, Department of Chemistry, Yale University, November 16, 2006.
4. "Possibility of novel gold-boron compounds", poster session, 232nd ACS National Meeting, San Francisco, CA, September 10-14, 2006.
5. "Peculiarities of chemical bonding in multiply charged silicon clusters: Joint ab-initio and photoelectron spectroscopy study", poster session, 231st ACS National Meeting, Atlanta, GA, March 26-30, 2006.