

Anastassia N. Alexandrova

Curriculum Vitae

*Department of Chemistry and Biochemistry
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Employment

- 2015-present** Associate Professor. University of California, Los Angeles, Department of Chemistry and Biochemistry, and California NanoSystems Institute
- 2016** Professeur Invité. École Normale Supérieure de Lyon, France
- 2016** Visiting Professor. ETH Zürich, Switzerland
- 2010-2015** Assistant Professor. University of California, Los Angeles, Department of Chemistry and Biochemistry, and California NanoSystems Institute

Education and Training

- 2008-2010** **Postdoctoral.** American Cancer Society Fellow, Department of Chemistry, Yale University (Advisor Dr. John C. Tully)
- 2005-2008** **Postdoctoral.** Department of Chemistry, Yale University (Advisor Dr. William L. Jorgensen)
- 2005** **Ph.D. in Physical Chemistry.** Department of Chemistry and Biochemistry, Utah State University (Advisor Dr. Alex I. Boldyrev)
- 2000-2001** **Predoctoral.** Vernadskii Institute of the Russian Academy of Sciences, Moscow, Russia (Advisor Dr. Lev A. Gribov)
- 2000** **B.S./M.S. in Chemistry.** *Summa cum laude.* Department of Chemistry, Saratov University, Russia.

Awards and Honors

- 2016** Fulbright Scholarship from the U.S.-France Commission
- 2015** The Rising Star Award of the Women Chemists Committee - American Chemical Society
- 2014** NSF CAREER Award
- 2014** Glenn T. Seaborg Award, recognizes outstanding achievements of early-career faculty in the Department of Chemistry & Biochemistry, UCLA
- 2014** Professor of the Year, UCLA BruinLife Yearbook
- 2013** Alfred P. Sloan Research Fellowship
- 2011** UCLA Faculty Career Development Award
- 2011** DARPA Young Faculty Award
- 2011** American Chemical Society YCC Leadership Development Award
- 2008-2009** Mary Fieser Postdoctoral Fellowship at Harvard - *declined*
- 2008-2010** American Cancer Society Postdoctoral Fellowship
- 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
- 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

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	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. DOE
2003-2004	National Deans' List
2003	The Chemistry and Biochemistry Alumni Research Award, Utah State University
2000	M.S. Honor Diploma (<i>Summa cum laude</i>)
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

Teaching

CHEM 113A, Introductory Quantum Mechanics
 CHEM 228, Physical chemistry seminar
 CHEM 189, Advanced Honors Seminar for CHEM 113A
 CHEM 126/226, Computational Methods for Chemists (laboratory)
 CHEM 208, Dissertation Seminar
 CHEM 20A, General Chemistry
 CHEM 89C, 89HC General Chemistry, honors elective and contract
 CHEM 20AH, Honors General Chemistry
 CHEM 115D/215D, Special Topics in Graduate Quantum
 CHEM 115A/215A, Graduate Quantum

Course development:

CHEM 126/226, Computational Methods for Chemists (laboratory), including the innovative final project that is a real research project done in the classroom. In 2012 and 2013, these resulted in publications with the students.

Professional Services

Editorial Activities:

2014-2016 Editorial Board: *Scientific Reports* (Nature Publishing Group)
2014-present Editorial Advisory Board: *Journal of Physical Chemistry* (ACS)

Affiliations, National Services:

American Chemical Society
 Chair of the Theory Subdivision of PHYS Division of the American Chemical Society (2015-2018)

Reviewing and review panel services:

NSF, PRF, DOE

Conducting scientific meetings:

2013-present Organizing (with Prof. Boldyrev) *Annual International Conference on Chemical Bonding (ICCB)*, Lihue, HI, USA. **The 2014 ICCB meeting highlighted in C&E News (Sept 22, 2014, pp 10-13) and featured on its cover.**
2014 Organizing (with Prof. Saeys) "Clusters in Catalysis" Symposium at the National ACS Meeting, Dallas, TX, USA

- 2013 Organizing and chairing the “Chemistry in Silico” part of the Transatlantic Frontiers of Chemistry symposium. Kloester Seeon, Germany.
- 2012 Discussion Leader at the International Conference of Young Researchers on Advanced Materials, in the category “Materials for Energy and the Environment”, Singapore.
- 2012 Organizing and chairing the Theory Section at the Gordon Research Conference – Catalysis, New London, NH, USA
- 2012 Organizing (with Prof. Houk) the “Quantum Mechanics and Molecular Dynamics of Chemical and Biological Reactivity” meeting, satellite to the International Congresses of Quantum Chemistry, Los Angeles, CA, USA
- 2004 Abstract management and web-design for the Regional ACS Meeting of the Northwest / Rocky Mountains Sections, Logan, UT, USA
-

Publications

H-index = 22, average citation per paper = 25.

81. Lei, J.; Yeung, M. T.; Robinson, P. J.; Mohammadi, R.; Turner, C. L.; Alexandrova, A. N.; Kavner, A.; Kaner, R.; Tolbert, S. H. *Volumetric deformation and strength anisotropy of orthorhombic tungsten monoboride under non-hydrostatic compression*. **2016**, in preparation.
80. Fuhr, A.; Shen, L.; Wang, X.; Alexandrova, A. N.; Lu, Y. *Solid-like Biomimetic Ion-Channel Electrolytes for Lithium Metal Batteries*. **2016**, in preparation.
79. Robinson, P.J.; Zhang, X.; McQueen, T.; Bowen, K. H.; Alexandrova, A. N. *Extreme Fluxionality of Charge in Sm-B Systems: Hypothesis Regarding the Mechanism for Mixed Valency in Kondo Insulator, SmB₆?* **2016**, in preparation.
78. Jimenez-Izal, E.; Saeys, M.; Alexandrova, A. N. *Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N*. **2016**, submitted.
77. Thomas, J. C.; Serino, A. C.; Goronzy, D. P.; Auluck, H. S.; Irving, O.; Jimenez-Izal, E.; Deirmenjian, J. M.; Alexandrova, A. N.; Baše, T.; Weiss, P. S. *Acid-Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can*. **2016**, in preparation.
76. Messina, M.; Axtell, J.; Wang, Y.; Chong, P.; Wixtrom, A.; Kirlikovali, K.; Upton, B.; Hunter, B.; Shaafat, O.; Khan, S.; Winkler, J.; Gray, H.; Alexandrova, A. N.; Maynard, H. D.; Spokoyny, A. M. *Visible Light-Induced Olefin Activation Using 3D Aromatic Boron-Rich Cluster Photooxidants*. *J. Am. Chem. Soc.* **2016**, DOI: 10.1021/jacs.6b03568.
75. Valdez, C. E.; Shirvanyants, D.; Dokholyan, N. V.; Alexandrova, A. N. *Eris-QM/DMD: a metalloprotein design tool*. **2016**, Submitted.
74. Gallup, N. M.; Alexandrova, A. N. *Use of QM/DMD as a Multiscale Approach to Modeling Metalloenzymes*. **2016**, Submitted.
73. Nechay, M. R.; Gallup, N. M.; Smith, Q. A.; Morgenstern, A.; Eberhart, M. E.; Alexandrova, A. N. *Histone Deacetylase 8: Characterization of Physiological Divalent Metal Catalysis*. *J. Phys. Chem. B* **2016**, William Gelbart Festschrift issue, DOI: 10.1021/acs.jpcc.6b00997.
72. Ha, M.-A.; Alexandrova, A. N. *Oxygen Vacancies of Anatase 101: Extreme Sensitivity to the Density Functional Theory Method*. *J. Chem. Theor. Comput.* **2016**, accepted.
71. Valdez, C. E.; Morgenstern, A.; Eberhart, M.; Alexandrova, A. N. *Computational Redesign of Carboxypeptidase A*. **2016**, Submitted.
70. Jimenez-Izal, E.; Alexandrova, A. N. *σ -Aromaticity in Polyhydride Complexes of Ir, Os, and Pt*. *Phys. Chem. Chem. Phys.* **2016**, 18, 11644–11652, **Invited article for the special issue on aromaticity**.

69. Robinson, P. J.; Alexandrova, A. N. *Assessing the bonding properties of individual molecular orbitals*. *J. Phys. Chem. A* **2015**, *119*, 12862–12867.
68. Qiu, J.; Zeng, G.; Ha, M.-A.; Hou, B.; Mechlenburg, M.; Shi, H.; Alexandrova, A. N.; Cronin, S. B. *Microscopic Study of Atomic Layer Deposition of TiO₂ on GaAs and its Photocatalytic Application*. *Chem. Mater.* **2015**, *27*, 7977–7981.
67. Qiu, J.; Zheng, G.; Ha, M.-A.; Ge, M.; Lin, Y.; Hettick, M.; Alexandrova, A. N.; Javey, A.; Cronin, S. B. *Artificial Photosynthesis on TiO₂-Passivated InP Nanopillars*. *Nano Lett.* **2015**, *15*, 6177–6181.
66. Zhang, X.; Robinson, P. J.; Gantefoer, G.; Alexandrova, A. N.; Bowen, K. H. *Photoelectron Spectroscopic and Theoretical Study of the [HPd(η^2 -H₂)] Cluster Anion*. *J. Chem. Phys.* **2015**, *143*, 094307.
65. Dadras, J.; Jimenez-Izal, E.; Alexandrova, A. N. *Alloying Pt Sub-Nano-Clusters with Boron: Sintering Preventative and Coke Antagonist?* *ACS Catal.* **2015**, *5*, 5719-5727.
64. Nandula, A.; Trinh, Q. T.; Saeys, M.; Alexandrova, A. N. *Origin of Extraordinary Stability of Square Planar Carbon in Surface Carbides of Co and Ni*. *Angew. Chem. Int. Ed.* **2015**, *54*, 5312-5316, **VIP article**.
63. Zhai, H.; Ha, M.-A.; Alexandrova, A. N. *AFFCK: Adaptive Force Field-Assisted ab initio Coalescent Kick Method for Global Minimum Search*. *J. Chem. Theor. Comput.* **2015**, *11*, 2385-2393.
62. Mouse, G.; Gallup, N. M.; Alexandrova, A. N.; Hengge, A. C.; Johnson, S. J. *Conservative tryptophan mutants of the protein-tyrosine phosphatase YopH exhibit impaired WPD-loop function and crystallize with divanadate esters in their active sites*. *Biochemistry* **2015**, *54*, 6490-6500.
61. Nechay, M. R.; Valdez, C. E.; Alexandrova, A. N. *Computational Treatment of Metalloenzymes*. *J. Phys. Chem. B* **2015**, *119*, 5945-5956, **Feature Article, Journal Cover**.
60. Dadras, J.; Shen, L.; Alexandrova, A. N. *Computational Study of Pt-Zn Clusters on Stoichiometric MgO(100) and TiO₂(110): Dramatically Different Sintering Behavior*. *J. Phys. Chem. C*, **2015**, *119*, 6047-6055.
59. Alexandrova, A. N.; Bouchard, L.-S. *Sub-Nano Clusters: the Last Frontier of Inorganic Chemistry*. *Adv. Chem. Phys.* **2015**, *156*, pp. 73-100. Eds.: S. A. Rice, A. R. Dinner, John Wiley & Sons Inc. Hoboken, NJ. ISBN: 978-1-118-94969-6. **Invited article**.
58. Nedd, S.; Alexandrova, A. N. *Pd-catalyzed Formation of Coumarin Proceeds via the Concerted Metalation-Deprotonation Mechanism. A Theoretical Study*. *Phys. Chem. Chem. Phys.* **2015**, *17*, 1347-1353.
57. Li, Z.; Gibson, R.; Le, T.; Poddar, S.; Smith, Q. A.; Santriero, B. D.; Czernin, J.; Alexandrova, A. N.; Jung, M. E.; Radu, C. C.; Lavie, A. *Structure-guided development of deoxycytidine kinase inhibitors with nanomolar affinity and improved metabolic stability*. *J. Med. Chem.* **2014**, *57*, 9480-9494.
56. Valdez, C. E.; Nechay, M. R.; Smith, T.; Alexandrova, A. N. *Mysteries of metals in metalloenzymes*. *Acc. Chem. Res.* **2014**, *47*, 3110-3117. **Invited article**.
55. Ha, M.-A.; Dadras, J.; Alexandrova, A. N. *Rutile-deposited PtPd clusters: a hypothesis about the special stability at 50/50 ratio*. *ACS Catal., special issue*, **2014**, *4*, 3570-3580. **Invited article for the special virtual issue on computational catalysis**.
54. Nedd, S.; Redler, R.; Proctor, E. A.; Dokholyan, N. V.; Alexandrova, A. N. *Cu,Zn-Superoxide Dismutase without Zn is Folded but Catalytically Inactive*. *J. Mol. Biol.* **2014**, *426*, 4112-4124.
53. Shen, L.; Dadras, J.; Alexandrova, A. N. *Pure and Zn-Doped Pt Clusters Go Flat and Upright on MgO(100)*. *Phys. Chem. Chem. Phys., special issue*, **2014**, *16*, 264366-26442. **Invited article. Featured on the Journal Cover**.
52. Valdez, C. E.; Gallup, N. M.; Alexandrova, A. N. *Co²⁺ Acireductone Dioxygenase: Fe²⁺ Mechanism, Ni²⁺ Mechanism, or Something Else?* *Chem. Phys. Lett.* **2014**, *604*, 77-82.

51. Zhang, X.; Bowen, K. H.; Alexandrova, A. N. *The PtAl⁻ and PtAl₂⁻ Ions: Theoretical and Photoelectron Spectroscopic Characterization*. *J. Chem. Phys.* **2014**, *140*, 164316.
50. Zhang, X.; Liu, G.; Gantefoer, G.; Bowen, K. H.; Alexandrova, A. N. *PtZnH₅⁻, a σ -aromatic cluster*. *J. Phys. Chem. Lett.* **2014**, *5*, 1596-1601. **Highlighted in Chemistry World, UK.**
49. Alexandrova, A. N.; Huber, S. M.; Tavasoli, A. *The 3rd Transatlantic Frontiers in Chemistry Symposium. Editorial*. *Chem. Eur. J.* **2013**, *19*, 15777-15783.
48. Alexandrova, A. N.; Nechay, M. R.; Lydon, B. R.; Buchan, D. P.; Yeh, A. J.; Tai, M.-H.; Kostrikin, I. P.; Gabrielyan, L. *The Same in the Bulk but Different as Clusters: X₃Y₃ (X = B, Al, Ga; Y = P, As)*. *Chem. Phys. Lett.* **2013**, *588*, 37-42.
47. Murphy, J. M.; Armijo, A. L.; Lee, C. H.; Campbell, D. O.; Li, Z.; Liao, H.-I.; Lee, J. T.; Nathanson, D.; Austin, W. R.; Nomme, J.; Darvish, R.; Smith, T.; Herschman, H. R.; Alexandrova, A. N.; Sadeghi, S.; Phelps, M. E.; Lavie, A.; Jung, M. E.; Czernin, J.; Satyamurthy, N.; Radu, C. G. *Development of new deoxycytidine kinase inhibitors and non-invasive in vivo evaluation using Positron Emission Tomography*. *J. Med. Chem.* **2013**, *56*, 6696-6708.
46. Zhang, J.; Alexandrova, A. N. *The Golden Crown: How a Single Gold Atom Boosts the CO Oxidation Catalyzed by Palladium Cluster on Titania Surfaces*. *J. Phys. Chem. Lett.* **2013**, *4*, 2250-2255.
45. Sparta, M.; Valdez, C. E.; Alexandrova, A. N. *Metal-dependent functionality of Fe and Ni acireductone dioxygenases: how extra two electrons reroute the catalytic pathway*. *J. Mol. Biol.* **2013**, *425*, 3007-2018. **Featured on the Journal Cover.**
44. Baraldi, C.; Freguglia, G.; Tinti, A.; Sparta, M.; Alexandrova, A. N.; Gamberini, M. C. *IR, Raman and SERS spectra of propantheline bromide*. *Spec. Acta A: Mol. Biomol. Spec.* **2013**, *103*, 1-10.
43. Valdez, C. E.; Sparta, M.; Alexandrova, A. N. *The role of the flexible L43-S54 protein loop of the CcrA metallo- β -lactamase in binding structurally dissimilar β -lactam antibiotics*. *J. Chem. Theor. Comput.* **2013**, *9*, 730-737.
42. Schmidt, N. W.; Lis, M.; Zhao, K.; Lai, G. H.; Alexandrova, A. N.; Tew, G. N.; Wong, G. L. *Molecular basis for nanoscopic membrane curvature generation from quantum mechanical models and synthetic transporter sequences*. *J. Am. Chem. Soc.* **2012**, *134*, 19207-19216.
41. Sparta, M.; Alexandrova, A. N. *How metal substitution affects the enzymatic activity of catechol-O-methyl transferase*. *PLoS ONE* **2012**, *7*, e47172.
40. Ramachandran, S.; Temple, B.; Alexandrova, A. N.; Chaney, S. G.; Dokholyan, N. V. *Recognition of Platinum-DNA adducts by HMGB1a*. *Biochemistry* **2012**, *51*, 7608-7617.
39. Valdez, C. E.; Alexandrova, A. N. *Why Urease is a di-Nickel Enzyme, whereas the CcrA β -Lactamase is a di-Zinc Enzyme*. *J. Phys. Chem. B* **2012**, *116*, 10649-10656. **Highlighted in C&E News.**
38. Kuznetsov, V. I.; Alexandrova, A. N.; Hengge, A. C. *Metavanadate at the active site of the phosphatase VHZ*. *J. Am. Chem. Soc.* **2012**, *134*, 14298-14301, **Editor's Spotlight article.**
37. Alexandrova, A. N.; Nayhouse, M. J.; Huynh, M. T.; Kuo, J. L.; Melkonian, A. V.; Chavez, G. De J.; Hernando, N. M.; Kowal, M. D.; Liu, C.-P. *AB₄^{2-/} (A = C, Si, Ge; B = Al, Ga, In) Ions: A Battle between Covalency and Aromaticity, and Prediction of Square Planar Si in SiIn₄^{2-/}*. *Phys. Chem. Chem. Phys.* **2012**, *14*, 14815-14821. **Invited article. Featured on the Journal Cover. Highlighted in UCLA Today.**
36. Zhang, J.; Sergeeva, A. P.; Sparta, M.; Alexandrova, A. N. *Photo-driven Molecular Wankel Engine, B₁₃⁺*. *Angew. Chem. Int. Ed.* **2012**, *51*, 8512-8515. **VIP article. Highlighted in Nature Nanotechnology, Chemistry World, Angew. Chem. (2012, 51, 2-4), NextBigFuture.com, PDAON.com, lenta.ru, Technology Review, and other media worldwide.**
35. Sparta, M.; Shirvanyants, D.; Ding, F.; Dokholyan, N. V.; Alexandrova, A. N. *Hybrid dynamics simulation engine for metalloproteins*. *Biophys. J.* **2012**, *103*, 767-776.

34. Alexandrova, A. N. *Tug of war between AO-hybridization and aromaticity in dictating structures of Li-doped alkali clusters*. *Chem. Phys. Lett.* **2012**, 533, 1-5. **Editor's Choice article. Featured on the Journal Cover.**
33. Zhang, J.; Alexandrova, A. N. *Double σ -Aromaticity in a Surface Deposited Cluster: Pd₄ on TiO₂ (110)*. *J. Phys. Chem. Lett.* **2012**, 3, 751-754.
32. Alexandrova, A. N. *Quantum Mechanical Insights into Biological Processes at the Electronic Level*. In *Computational Modeling of Biological Systems: From Molecules to Pathways*, Springer Science+Business Media, LLC, **2012**, ISSN 1618-7210; ISBN 978-1-4614-2145-0; DOI 10.1007/978-1-4614-2146-7, pp. 117-164.
31. Alexandrova, A. N.; Jorgensen, W. L. *On the Mechanism and Rate of Spontaneous Decomposition of Amino Acids*. *J. Phys. Chem. B* **2011**, 115, 13624-13632.
30. Zhang, J.; Alexandrova, A. N. *Structure, stability, and mobility of small Pd clusters on the stoichiometric and defective TiO₂ (110) surfaces*. *J. Chem. Phys.* **2011**, 135, 174702. **Chosen for the Virtual Journal of Nanoscale Science & Technology, 2011, 24, 20.**
29. Huynh, M. T.; Alexandrova, A. N. *Persistent Covalency and Planarity in the B_nAl_{6-n}²⁻ and LiB_nAl_{6-n}⁻ (n=1-6) Cluster Ions*. *J. Phys. Chem. Lett.* **2011**, 2, 2046-2051.
28. Sparta, M.; Alexandrova, A. N. *Computational design and characterization of artificial enzymes for Kemp elimination*. *Mol. Sim.* (Recent Advances in Molecular Simulation, special issue) **2011**, 37, 557-571, **Invited article.**
27. Shirvanyants, D.; Alexandrova, A. N.; Dokholyan, N. V. *Rigid substructure search*. *Bioinformatics* **2011**, 27, 1327-1329.
26. Alexandrova, A. N.; Boldyrev, A. I.; Li, X.; Sarkas, H. W.; Hendricks, J. H.; Arnold, S. T.; Bowen, K. H. *Lithium Cluster Anions: Photoelectron Spectroscopy and Ab Initio Calculations*. *J. Chem. Phys.* **2011**, 134, 044322.
25. Alexandrova, A. N. *H•(H₂O)_n Clusters – Microsolvation of the Hydrogen Atom via Molecular ab initio Gradient Embedded Genetic Algorithm (GEGA)*. *J. Phys. Chem. A* **2010**, 114, 12591–12599.
24. Alexandrova, A. N. *Promiscuous DNA Alkyladenine Glycosylase Dramatically Favors a Bound Lesion Over Undamaged Adenine*. *Biophys. Chem.* **2010**, 152, 118-127.

Postdoctoral work at Yale:

23. Alexandrova, A. N.; Tully, J. C.; Granucci, G. *Photochemistry of DNA Fragments via Semiclassical Nonadiabatic Dynamics*. *J. Phys. Chem. B* **2010**, 114, 12116–12128.
22. Bopp, J. C.; Alexandrova, A. N.; Elliott, B. M.; Herden, T.; Johnson, M. A. *Infrared vibrational spectra of On⁻ 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. Alexandrova, A. N.; Jorgensen, W. L. *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. Alexandrova, A. N.; Roethlisberger, D.; Baker, D.; Jorgensen, W. L. *Catalytic Mechanism and Performance of Computationally Designed Enzymes for Kemp Elimination*. *J. Am. Chem. Soc.* **2008**, 130, 15907-15915.
19. Jorgensen, W. L.; Jensen, K. P.; Alexandrova, A. N. *Polarization Effects for Hydrogen-Bonded Complexes of Substituted Phenols with Water*. *J. Chem. Theor. Comput.* **2007**, 3, 1987-1992.
18. Alexandrova, A. N.; Jorgensen, W. L. *Why Urea Eliminates Ammonia Rather Than Hydrolyzes in Aqueous Solution*. *J. Phys. Chem. B* **2007**, 111, 720-730.

Graduate work at USU:

17. Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. *All-Boron Aromatic Clusters as Potential New Inorganic Ligands and Building Blocks in Chemistry. Coord. Chem. Rev.* **2006**, *250*, 2811.
16. Zubarev, D. Yu.; Alexandrova, A. N.; Boldyrev, A. I.; Cui, L.-F.; Li, X.; Wang, L.-S. *On the Structure and Chemical Bonding of Si_6^{2-} and Si_6^{2-} in $NaSi_6^-$ Upon Na^+ Coordination. J. Chem. Phys.* **2006**, *124*, 124305.
15. Alexandrova, A. N.; Koyle, E.; Boldyrev, A. I. *Theoretical Study of Hydrogenation of Doubly-Aromatic B_7^- . J. Mol. Model.* **2006**, *12*, 569-576.
14. Alexandrova, A. N.; Boldyrev, A. I. *Search for the $Li_x^{0/+1/-1}$ Lowest Energy Structures Using Ab Initio Gradient Embedded Genetic Algorithm (GEGA). Elucidation of the Chemical Bonding in the Lithium Clusters. J. Chem. Theory Comput.* **2005**, *1*, 566-580.
13. Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. *Doubly-Antiaromatic All-Boron Ligand B_6^{2-} in the LiB_6^- molecule. Ab Initio and Photoelectron Spectroscopic Study. J. Chem. Phys.* **2005**, *122*, 054313.
12. Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. *$Cu_3C_4^-$ - a New Sandwich Molecule with Two Revolving C_2^{2-} Units. J. Phys. Chem. A* **2005**, *109*, 562, **Featured on the Journal Cover.**
11. Alexandrova, A. N.; Boldyrev, A. I.; Fu, Y.-J.; Yang, X.; Wang, X.-B.; Wang, L.-S. *Structure of the $Na_xCl_{x+1}^-$ ($x=1-4$) Clusters via Ab Initio Genetic Algorithm and Photoelectron Spectroscopy. J. Chem. Phys.* **2004**, *121*, 5709.
10. Alexandrova, A. N.; Zhai, H.-J.; Wang, L.-S.; Boldyrev, A. I. *Molecular Wheel B_8^{2-} as a New Inorganic Ligand: Photoelectron Spectroscopy and Ab Initio Characterization of the LiB_8^- Anion. Inorg. Chem.* **2004**, *43*, 3552.
9. Alexandrova, A. N.; Boldyrev, A. I. *Arachno-, Nido- and Closo-Aromatic Isomers of the $Li_6B_6H_6$ Molecule. Inorg. Chem.* **2004**, *43*, 3588.
8. Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. *Electronic Structure, Isomerism, and Chemical Bonding in B_7^- and B_7 . J. Phys. Chem. A* **2004**, *108*, 3509.
7. Zhai, H.-J.; Alexandrova, A. N.; Boldyrev, A. I.; Boldyrev, A. I. *Hepta- and Octacoordinate Boron in Molecular Wheels of Eight- and Nine-Atom Boron Clusters: Observation and Confirmation. Angew. Chem. Int. Ed.* **2003**, *42*, 6004.
6. Zhai, H.-J.; Wang, L.-S.; Alexandrova, A. N.; Boldyrev, A. I.; Zakrzewski, V. *Photoelectron Spectroscopy and Ab Initio Study of B_3^- and B_4^- Anions and Their Neutrals. J. Phys. Chem. A* **2003**, *107*, 9319.
5. Alexandrova, A. N.; Birch, K. A.; Boldyrev, A. I. *Flattening the $B_6H_6^{2-}$ Octahedron. Ab Initio Prediction of the New Family of Planar All-Boron Aromatic Molecules. J. Am. Chem. Soc.* **2003**, *125*, 10786.
4. Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S.; Steiner, E.; Fowler, P. W. *Structure and Bonding in B_6^- and B_6 : Planarity and Antiaromaticity. J. Phys. Chem. A* **2003**, *107*, 1359.
3. Elliott, B. M.; Alexandrova, A. N.; Boldyrev, A. I. *Hydrogen Trioxide Anion: A Possible Atmospheric Intermediate and Path of Oxygen-Rich Molecules. J. Phys. Chem. A* **2003**, *107*, 1203.
2. Alexandrova, A. N.; Boldyrev, A. I. *σ -Aromaticity and σ -Antiaromaticity in Alkaline Metal and Alkaline Earth Metal Small Clusters. J. Phys. Chem. A* **2003**, *107*, 554.
1. Zhai, H.-J.; Wang, L.-S.; Alexandrova, A. N.; Boldyrev, A. I. *Electronic Structure and Chemical Bonding of B_5^- and B_5 by Photoelectron Spectroscopy and Ab Initio Calculations. J. Chem. Phys.* **2002**, *117*, 7917.

Presentations at Professional Meetings

2017:

(Oral, Invited) Spring National ACS Meeting, Symposium “Quantum Dynamics in Large Scale Systems”, San Francisco, CA

(Oral, Invited) Spring MRS Meeting, Symposium “MGI Approaches to Accelerated Materials Discovery”, Phoenix, AZ

(Oral, Invited) American Conference on Theoretical Chemistry, Boston, MA

2016:

(Oral, Invited) Fall National ACS Meeting, Symposium “Advanced Potential Energy Surfaces”, Philadelphia, PA

(Oral) 4th International Conference on Chemical Bonding, Lihue, HI

(Oral, Invited) Rencontres des Chimistes Théoriciens Francophones (RCTF2016), Lyon, France

(Oral) 16th International Conference on Theoretical Aspects of Catalysis, Zakopane, Poland

(Oral, Invited) Multiscale Modelling of Condensed Phase and Biological Systems, Manchester, UK

(Invited Keynote Lecture) Spring National ACS Meeting, Symposium “Computational Chemistry Across Catalysis”, San Diego, CA

(Oral, Invited) Spring National ACS Meeting, Symposium WCC ACS Award Symposium, San Diego, CA

(Oral, Invited) Spring National ACS Meeting, Symposium “Catalysis at the Sub-Nanometer Scale”, San Diego, CA

(Oral, Invited) Spring National ACS Meeting, Symposium “Computational Materials Chemistry”, San Diego, CA

(Oral, Invited) Gordon Research Conference: Metals in Biology, Ventura, CA

2015:

(Oral, Invited) Pacifichem 2015, Symposium “Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities”, Honolulu, HI

(Oral, Invited) John Tully Retirement Symposium, Yale University, New Haven, CT

(Oral, Invited) Fall National ACS Meeting, Symposium “Physical Chemistry of Clusters and Nanoparticles”, Boston, MA

(Oral) 3rd International Conference on Chemical Bonding, Lihue, HI

(Oral, invited) Symposium honoring Jack Simons’ 70th Birthday. Salt lake City, UT

(Oral, invited) Symposium for the 43rd John Stauffer Distinguished Lecture in the Sciences honoring Prof. George Schatz, Los Angeles, CA

(Oral, Invited) Spring National ACS Meeting, Symposium dedicated to Don Truhlar, Denver, CO

2014:

(Oral, Invited) New Approaches to Materials Design, Moscow, Russia

(Oral) AIChE Annual Meeting, Atlanta, GA

(Oral, Invited) WATOC, Santiago, Chili

(Oral) 2nd International Conference on Chemical Bonding, Lihue, HI

(Oral, Invited) Gordon Research Conference: Atomic and Molecular Interactions, Stonehill College, Easton, MA

(Oral, Invited) Clusters, nanoparticles and nanostructures in catalysis and beyond, Mini-symposium, Computational Material Science Laboratory of the Institute of Theoretical and Computational Chemistry (IQTUCB), Universitat de Barcelona, Barcelona, Spain

(Oral, Invited) XI Girona Seminar on Carbon, Metal, and Carbon-Metal Clusters: From Theory to Applications, Girona, Spain

2013:

(Oral, Invited) AIChE Annual Meeting, San Francisco, CA

(Oral, Invited) Transatlantic Frontiers of Chemistry. Kloster Seon, Germany
(Oral) 1st International Conference on Chemical Bonding, Lihue, HI
(Oral, Invited) Workshop on Multiscale Theory and Simulation, Chicago, IL
(Poster) North American Catalysis Society Meeting, Louisville, KY
(Poster) Gordon Research Conference, Chemical Reactions at Surfaces, Les Diablerets, Switzerland
(**Invited Keynote Lecture**) 3rd Molecular Materials Meeting (M3), Singapore

2012:

(Oral, invited) 7th Singapore International Chemistry Conference (SICC-7). Singapore
(Oral, invited) Bridging the gap between ab initio and classical simulations, symposium at the 244th National ACS Meeting, Philadelphia, PA
(**Invited Keynote Lecture**) International Conference of Young Researchers on Advanced Materials, Singapore
(Oral, invited) Quantum Mechanics and Molecular Dynamics of Organic and Biological Reactivity, satellite to the ICQC, Los Angeles, CA
(Oral, invited) Nonadiabatic Dynamics: Surface Hopping and Beyond, special symposium dedicated to John Tully's 70th Birthday, the 243th National ACS Meeting, San Diego, CA

2011:

(Oral, invited) Understanding Chemical Reactivity through Computational Chemistry, symposium at the Western Regional American Chemical Society, Pasadena, CA
(Oral, invited) Building Bonds: A Joint China-U.S. Workshop for Women Researchers in Chemistry, Beijing, China
(Oral, invited) Navigating Chemical Compound Space for Materials and Bio Design, a long-term program at the UCLA Institute for Pure and Applied Mathematics.
(Oral, invited) CNSI-JAIST workshop, Los Angeles, CA

2010:

(Oral, invited) 240 National ACS meeting, John Tully 70th Birthday Symposium, Boston, MA
(Poster) Gordon Research Conference, New London, NH
(Poster) Biophysical Society Meeting, San Francisco

Before 2010:

(Oral, invited) Alexandrova, A. N.; Jorgensen, W. L. Protein Design Processes, Seattle, WA, September **2008**.
(Oral) Alexandrova, A. N.; Jorgensen, W. L. 236 National ACS Meeting, Philadelphia, PA, August **2008**.
(Poster) Alexandrova, A. N.; Jorgensen, W. L. American Conference on Theoretical Chemistry, Northwestern University, Evanston, IL, July **2008**.
(Oral, invited) Alexandrova, A. N.; Jorgensen, W. L. Protein Design Processes, Islamorada, FL, December **2007**.
(Poster, Invited) Alexandrova, A. N.; Jorgensen, W. L. Protein Design Processes, Islamorada, FL, December **2007**.
(Poster, invited) Alexandrova, A. N.; Jorgensen, W. L.; Baker, D. BSM Symposium, Yale University, August **2007**.
(Poster) Alexandrova, A. N.; Jorgensen, W. L.; Baker, D. 234th National ACS Meeting, Boston, MA, August **2007**.
(Oral, invited) Alexandrova, A. N.; Jorgensen, W. L. Protein Design Processes, Santa Fe, NM, June **2007**.
(Oral, invited) Alexandrova, A. N.; Jorgensen, W. L.; Baker, D. Northeastern Section YCC ACS Chemistry Research Conference, Boston, MA, April **2007**.

- (Online, invited) Alexandrova, A. N.; Jorgensen, W. L. The Electronic Computational Chemistry Conference, April, **2007**.
- (Oral, invited) Alexandrova, A. N.; Jorgensen, W. L. Protein Design Processes, Los Angeles, CA, January **2007**.
- (Poster) Alexandrova, A. N.; Jorgensen, W. L. Academic Employment Initiative, 232 National ACS Meeting, San Francisco, CA, September **2006**.
- (Poster) Alexandrova, A. N.; Jorgensen, W. L. 232 National ACS Meeting, San Francisco, CA, September **2006**.
- (Oral, invited) Alexandrova, A. N.; Tubert-Brohman, I.; Guimarães, C.; Jorgensen, W. L. Protein Design Processes, Islamorada, FL, April **2006**.
- (Poster, invited) Alexandrova, A. N.; Tubert-Brohman, I.; Guimarães, C.; Jorgensen, W. L. Protein Design Processes, Islamorada, FL, April **2006**.
- (Poster) Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. 229 National ACS Meeting, San Diego, CA, March **2005**.
- (Poster) Elliott, B. M.; Boldyrev, A. I.; Alexandrova, A. N.; Zhai, H.-J.; Yang, X.; Wang, X.-B.; Wang, L.-S. 229 National ACS Meeting, San Diego, CA, March **2005**.
- (Poster) Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. Winter School in Theoretical Chemistry, Helsinki, Finland, December **2004**.
- (Poster) Alexandrova, A. N.; Boldyrev, A. I. 85 Meeting of the AAAS Pacific Division, Logan, UT, June **2004**.
- (Poster) Alexandrova, A. N.; Boldyrev, A. I. 59 Joint Regional Meeting of the Northwest and Rocky Mountain Sections of the ACS, Logan, UT, June **2004**.
- (Poster) Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. 227 National ACS Meeting, Anaheim, CA, March **2004**.
- (Poster) Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. 20th Symposium on Molecular Structure, Austin, TX, March **2004**.
- (Poster) Elliott, B. M.; Boldyrev, A. I.; Alexandrova, A. N.; Zhai, H.-J.; Yang, X.; Wang, X.-B.; Wang, L.-S. 20th Symposium on Molecular Structure, Austin, TX, March **2004**.
- (Poster) Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. 225th National ACS Meeting, New Orleans, LA, USA. March **2003**.
- (Oral) Alexandrova, A. N.; Kozlova, L. M. B.S./M.S. Diploma Public Defense, June, **2000**.
- (Oral) Alexandrova, A. N.; Chernova, R. K. Undergraduate Student Conference, Saratov, Russia, May, **1998**.
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Invited Talks

2016:

University of Texas in Austin, Department of Chemistry
University of Colorado, Boulder, Department of Chemistry
University of Girona, Spain
ENS Lyon, Institute of Chemistry, France
EPFL Lausanne, Switzerland
University of Basel, Switzerland
ETH Zurich, Switzerland

2015:

Johns Hopkins University, Department of Chemistry

ENS Lyon, Institute of Chemistry, France
ETH Zurich, Switzerland
University of Nevada, Reno, Department of Chemistry
University of California, Riverside, College of Engineering
Brown University, Department of Chemistry
MIT-Harvard-BU, Greater-Boston-Area Theoretical Chemistry Seminar series (invited by students)
University of Wisconsin, Madison, Department of Chemistry

2014:

University of California, Berkeley, Department of Chemistry
University of Toronto, Department of Chemistry, Canada
University of Houston, Department of Chemistry

2013:

Ghent University, Center for Molecular Modeling, Belgium
Sorbonne University, the Laboratory of Theoretical Chemistry, Paris, France
University of Washington, Department of Chemistry
Colorado School of Mines, Department of Chemistry and Geochemistry
Rice University, Department of Chemistry
Marburg University, Germany
University of Amsterdam, Van't Hoff Institute for Molecular Sciences, Netherlands
Stanford University, Department of Chemistry
California Institute of Technology, Department of Chemistry
University of California, San Diego, Department of Chemistry
University of North Carolina at Chapel Hill, Department of Biochemistry and Biophysics

2012:

National University of Singapore, Department of Chemical Engineering
Unidad Mérida, Departamento de Física Aplicada, Mexico
University of Pittsburgh, Department of Chemistry
Northwestern University, Department of Chemistry
University of Chicago, James Franck Institute
University of California, Los Angeles, Department of Chemistry and Biochemistry
National University of Singapore, Department of Chemical Engineering

2011:

Utah State University, Department of Chemistry and Biochemistry
University of Southern California, Department of Chemistry

2010:

Arizona State University, Department of Chemistry
University of California, Berkeley, Department of Chemistry, Prof. William Lester group
California State University, Northridge, Department of Chemistry and Biochemistry

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
