

# 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

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### 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** **Predocctoral.** 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.

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### Awards and Honors

- 2018** Cottrell Scholars Collaborative Academic Leadership Training Workshop
- 2016** Hanson-Dow Award for Excellence in Teaching, UCLA
- 2016** Herbert Newby McCoy Award for excellence in faculty research, UCLA
- 2016** Fulbright Scholarship from the U.S.-France Commission - *declined*
- 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 (*Summa cum laude*)  
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

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## **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.

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## **Professional Services**

### **Editorial Activities:**

2014-2016 Editorial Board: *Scientific Reports* (Nature Publishing Group)  
2014-2016 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. Alexander Boldyrev) *Annual International Conference on Chemical Bonding (ICCB)*, Lihue, HI, USA.  
**The 2014 and 2016 ICCB highlighted in C&E News** (Sept 22, 2014, pp 10-13 – cover article; Oct 17, 2016, pp 21-25), **ACS Cent. Sci.** (DOI 10.1021/acscentsci.6b00337), and **JPC A** (DOI: 10.1021/acs.jpca.6b11179)
- 2019** Organizing (with Prof. Benjamin Schwartz) the SoCal TheoChem 4.0 Symposium, UCLA, Los Angeles, CA
- 2018** Organizing (with Prof. Eva Zurek) the “Materials in extreme environments” symposium at the National ACS Meeting, Boston, MA, USA
- 2018** Organizing (with Prof. Philippe Sautet) 17<sup>th</sup> International Conference of Theoretical Aspects of Catalysis (ICTAC), Los Angeles, CA
- 2018** Advisory Board member of the Latin American Conference on Chemical Bonding, Brazil
- 2018** Organizing (with Prof. Michael White) a “Supported sub-nano clusters as the smallest and highly tunable interface for chemistry” symposium at the American Physical Society meeting, Los Angeles, CA
- 2014** Organizing (with Prof. Mark 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. Kloster 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 = 25, total citations = 2861, average citation per article = 27 – April 2018)**

98. Halder, A.; Ha, M.-A.; Zhai, H.; Yang B.; Pellin, M. J.; Seifert, S.; Vajda, S.; Alexandrova, A. N. *Dynamics Defines Selectivity of Subnanometer Cluster Catalysts: Oxidative Dehydrogenation of Cyclohexane on Pd versus Cu Clusters*. **2018**, submitted.
97. Shalhout, F. Y.; Malyk, S.; Hinman, J. G.; Cronin, S. B.; Jimenez-Izal, E.; Alexandrova, A. N.; Benderskii, A. V. *Water-Enhanced Carbon Monoxide Adsorption on Roughened Gold Surfaces in Ambient Conditions*. **2018**, under review.
96. Jimenez-Izal, E.; Zhai, H.; Alexandrova, A. N. *Nanoalloying MgO-Deposited Pt Clusters with Si for Controlling the Selectivity of Alkane Dehydrogenation*. **2018**, under review.
95. Zhai, H.; Alexandrova, A. N. *Local Fluxionality of Surface-Deposited Cluster Catalysts: the Case of Pt<sub>7</sub> on Al<sub>2</sub>O<sub>3</sub>*. *J. Phys. Chem. Lett.* **2018**, 9, 1696-1702.
94. Popov, I. A.; Jimenez-Izal, E.; Alexandrova, A. N.; Boldyrev, A. I. *Multicenter Bonding Effects in Oxygen Vacancy in Bulk and on the Surface of MgO*. **2018**, under review.
93. Dyck, O.; Kim, S.; Jimenez-Izal, E.; Alexandrova, A. N.; Kalinin, S. V.; Jesse, S. *Assembling Di- and Multiatomic Si Clusters in Graphene via Electron Beam Manipulation*. **2018**, under review, *arXiv:1710.09416 [cond-mat.mtrl-sci]*.

92. Huang, C.; Irving, O. R.; Alexandrova, A. N. *Oxidation Potentials of Class Ia Fe RNR and Class Ib Mn RNR in Escherichia Coli are Brought Close by the Protein Environment*. **2018**, under review.
91. Thomas, J. C.; Goronzy, D. P.; Serino, A. C.; Auluck, H. S.; Irving, O. R.; Jimenez-Izal, E.; Deirmenjian, J. M.; Macháček, J.; Sautet, P.; Alexandrova, A. N.; Baše, T.; Weiss, P. S. *Acid-Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can*. *ACS Nano* **2018**, DOI: 10.1021/acsnano.7b09011.
90. Lei, J.; Yeung, M. T.; Robinson, P. J.; Mohammadi, R.; Turner, C. L.; Yan, J.; Kavner, A.; Alexandrova, A. N.; Kaner, R. B.; Tolbert, S. H. *Understanding How Bonding Controls Strength Anisotropy in Hard Materials by Comparing the High Pressure Behavior of Orthorhombic and Tetragonal Tungsten Monoboride*. *J. Phys. Chem. C* **2018**, 122, 5647-5656.
89. Jimenez-Izal, E.; Alexandrova, A. N. *Computational design of clusters for catalysis*. *Ann. Rev. Chem. Phys.* **2018**, 69, 377-400, invited article.
88. Baxter, E. T.; Ha, M.-A.; Cass, A. C.; Zhai, H.; Alexandrova, A. N.; Anderson, S. L. *Diborane Interactions with Pt<sub>7</sub>/alumina: Preparation of Size-Controlled Borated Pt Model Catalysts with Improved Coking Resistance*. *J. Phys. Chem. C* **2018**, 122, 1631-1644.
87. Robinson, P.J.; Zhang, X.; McQueen, T.; Bowen, K. H.; Alexandrova, A. N. *Mystery of Three Borides: Promiscuous Metal-Boron Bonding Governing Superhard Structures*. *Chem. Mater.* **2017**, 29, 9892-9896.
86. Alexandrova, A. N. *Divide-and-Conquer Chemical Bonding Models for Materials: a Tool for Materials Design at the Electronic Level*. *Chem. Mater.* **2017**, 29, 8555-8565, invited **"Up-and-Coming article", among the top-20 most downloaded papers of the month of October, 2017**.
85. Ha, M.-A.; Baxter, E. T.; Cass, A. C.; Anderson, S. L.; Alexandrova, A. N. *Boron Switch for Selectivity of Catalytic Dehydrogenation on Size-Selected Pt clusters on Al<sub>2</sub>O<sub>3</sub>*. *J. Am. Chem. Soc.* **2017**, 139, 11568-11575.
84. Morgenstern, A.; Jaszai, M.; Eberhart, M. E.; Alexandrova, A. N. *Quantified Electrostatic Preorganization in Enzymes Using the Geometry of the Electron Charge Density*. *Chem. Sci.* **2017**, 8, 5010-5018.
83. Baxter, E. T.; Ha, M.-A.; Cass, A. C.; Alexandrova, A. N.; Anderson, S. L. *Ethylene Dehydrogenation on Pt<sub>4,7,8</sub> clusters on Al<sub>2</sub>O<sub>3</sub>: Strong Cluster-Size Dependence Linked to Preferred Catalyst Morphologies*. *ACS Catal.* **2017**, 7, 3322-3335.
82. Cui, Z.; Jimenez-Izal, E.; Alexandrova, A. N. *Prediction of two-dimensional boron phase with anisotropic electrical conductivity*. *J. Phys. Chem. Lett.* **2017**, 8, 1224-1228.
81. Zhai, H.; Alexandrova, A. N. *Fluxionality of Catalytic Clusters: When It Matters and How to Address It*. *ACS Catal.* **2017**, 7, 1905-1911. **Viewpoint Article**.
80. Robinson, P.J.; Zhang, X.; McQueen, T.; Bowen, K. H.; Alexandrova, A. N. *SmB<sub>6</sub><sup>-</sup> Cluster Anion: Covalency Involving f-Orbitals*. *J. Phys. Chem. A* **2017**, 121, 1849-1854.
79. Ugalde, J. M.; Bultinck, P.; Bickelhaupt, F. M.; Alexandrova, A. N. *The 4th International Conference on Chemical Bonding*. *J. Phys. Chem. A* **2016**, 120, 9353-9356.
78. Zhai, H.; Alexandrova, A. N. *Ensemble-Average Representation of Pt clusters in Conditions of Catalysis Accessed through GPU Accelerated Deep Neural Network Fitting Global Optimization*. *J. Chem. Theor. Comput.* **2016**, 12, 6213-6226.
77. Jimenez-Izal, E.; Saeys, M.; Alexandrova, A. N. *Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N*. *J. Phys. Chem. C* **2016**, 120, Mark Gordon Festschrift Issue, 21685-21690.
76. Zhang, X.; Ganrefoer, G.; Alexandrova, A. N.; Bowen, K. *Photoelectron Spectroscopic and Computational Study of the PtMgH<sub>3,5</sub><sup>-</sup> Cluster Anions*. *Phys. Chem. Chem. Phys.* **2016**, 18, 19345-19349.

75. Messina, M. S.; Axtell, J. C.; Wang, Y.; Chong, P.; Wixtrom, A. I.; Kirlikovali, K. D.; Upton, B. M.; Hunter, B. M.; Shaafat, O. S.; Khan, S. I.; Winkler, J. R.; Gray, H. B.; 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**, *138*, 6952–6955. **Highlighted in Science** **2016**, *352*, 1422-1423.
74. Gallup, N. M.; Alexandrova, A. N. *Use of QM/DMD as a Multiscale Approach to Modeling Metalloenzymes*. In *Methods in Enzymology*, **2016**, *577*, 319-339.
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**, *120*, 5884-5895, William Gelbart Festschrift issue.
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**, *12*, 2889–2895.
71. Valdez, C. E.; Morgenstern, A.; Eberhart, M. E.; Alexandrova, A. N. *Predictive Methods for Computational Metalloenzyme Redesign - A Test Case with Carboxypeptidase A*. *Phys. Chem. Chem. Phys.* **2016**, *18*, 31744-31756.
70. Jimenez-Izal, E.; Alexandrova, A. N.  *$\sigma$ -Aromaticity in Polyhydride Complexes of Ru, 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.; Meclenburg, M.; Shi, H.; Alexandrova, A. N.; Cronin, S. B. *Microscopic Study of Atomic Layer Deposition of TiO<sub>2</sub> 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.; Hou, B.; Alexandrova, A. N.; Javey, A.; Cronin, S. B. *Artificial Photosynthesis on TiO<sub>2</sub>-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( $\eta^2$ -H<sub>2</sub>)] 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 Atoms in Surface Carbides of Cobalt and Nickel*. *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. Moise, 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 Metalloproteins*. *J. Phys. Chem. B* **2015**, *119*, 5945-5956, **Feature Article, Journal Cover**.
60. Dadras, J.; Shen, L.; Alexandrova, A. N. *Pt-Zn Clusters on Stoichiometric MgO(100) and TiO<sub>2</sub>(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. *The Mechanism of Pd-catalyzed Formation of Coumarin: A Theoretical Study*. *Phys. Chem. Chem. Phys.* **2015**, *17*, 1347-1353.

57. Nomme, J.; Li, Z.; Gibson, R. M.; Wang, J.; Armijo, A. L.; Le, T.; Poddar, S.; Smith, T.; Santarsiero, B. D.; Nguyen, H.-A.; Czernin, J.; Alexandrova, A. N.; Jung, M. E.; Radu, 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. *Co<sup>2+</sup> Acireductone Dioxygenase: Fe<sup>2+</sup> Mechanism, Ni<sup>2+</sup> Mechanism, or Something Else?* *Chem. Phys. Lett.* **2014**, *604*, 77-82.
51. Zhang, X.; Bowen, K. H.; Alexandrova, A. N. *The PtAl<sup>-</sup> and PtAl<sub>2</sub><sup>-</sup> 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. *PtZnH<sub>5</sub><sup>-</sup>, a  $\sigma$ -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 3<sup>rd</sup> 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: X<sub>3</sub>Y<sub>3</sub> (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- $\beta$ -lactamase in binding structurally dissimilar  $\beta$ -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  $\beta$ -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.  *$AB_4^{2-/}$  ( $A = C, Si, Ge$ ;  $B = Al, Ga, In$ ) Ions: A Battle between Covalency and Aromaticity, and Prediction of Square Planar Si in  $SiIn_4^{2-/}$* . *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,  $B_{13}^+$* . *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  $\sigma$ -Aromaticity in a Surface Deposited Cluster:  $Pd_4$  on  $TiO_2$  (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  $TiO_2$  (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.  *$H\cdot(H_2O)_n$  Clusters – Microsolvation of the Hydrogen Atom via Molecular ab initio Gradient Embedded Genetic Algorithm (GEGA)*. *J. Phys. Chem. A* **2010**, *114*, 12591–12599. **Featured in the JPC Collection of works by prominent female physical chemists, in dedication to the 150<sup>th</sup> Birthday of Marie Curie**, <http://pubs.acs.org/page/vi/jpc-mariecurie>
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.  *$\sigma$ -Aromaticity and  $\sigma$ -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.
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## **Presentations at Professional Meetings**

### **2018:**

- (Oral) 6<sup>th</sup> International Conference on Chemical Bonding, Lihue, HI
- (Oral, Invited) International Congress of Quantum Chemistry (ICQC), Menton, France
- (Oral, Invited) CECAM workshop on modeling metals in materials science, Paris, France
- (Oral, Invited) Spring National ACS Meeting, Symposium "Insights into Structure, Function, Dynamics and Evolution of Enzymatic Mechanisms from Computational Simulation", New Orleans, LA
- (Oral, Invited) Spring National ACS Meeting, Symposium "Activation of light (C1-C4) hydrocarbons. Theory and experiments", New Orleans, LA

### **2017:**

- (Oral, Invited) "Optimization and Optimal Control for Complex Energy and Property Landscapes" Workshop, IPAM, UCLA, Los Angeles, CA
- (Oral, Invited) Fall National ACS Meeting, Symposium "Metal-support Interactions", Washington DC
- (Oral, Invited) Fall National ACS Meeting, Symposium "Experimental and Computational Advances in Understanding Enzyme Specificity and Promiscuity", Washington DC
- (Oral, Invited) Fall National ACS Meeting, Symposium "New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics", Washington DC
- (Oral, Invited) American Conference on Theoretical Chemistry, Boston, MA
- (Oral) 5<sup>th</sup> International Conference on Chemical Bonding, Lihue, HI
- (Oral, Invited) SoCal Theochem 2.0, UC Irvine, Irvine, CA
- (Oral, Invited) Spring MRS Meeting, Symposium "MGI Approaches to Accelerated Materials Discovery", Phoenix, AZ
- (Oral, Invited) Spring National ACS Meeting, Symposium "Quantum Dynamics in Large Scale Systems", San Francisco, CA
- (Oral, Invited) Spring National ACS Meeting, Symposium "Catalytic Materials from Molecular Insight", San Francisco, CA – **Chosen as the Best Presentation of the session**
- (Oral, Invited) Spring National ACS Meeting, Symposium "Methods for Modeling Materials Chemistry", San Francisco, CA
- (Oral, Invited) Sustainable Chemistry/ACAI Net meeting, UCSB, Santa Barbara, CA

**2016:**

- (Oral, Invited) Workshop “Collective Variables in Quantum Mechanics”, Institute for Pure and Applied Mathematics (IPAM), UCLA
- (Oral, Invited) Fall National ACS Meeting, Symposium “PHYS: Advanced Potential Energy Surfaces”, Philadelphia, PA
- (Oral, Contributed) Fall National ACS Meeting, Symposium “COMP: Materials Chemistry”, Philadelphia, PA
- (Oral, Contributed) Fall National ACS Meeting, Symposium “CATL: Computational Catalysis”, Philadelphia, PA
- (Oral) 4<sup>th</sup> International Conference on Chemical Bonding, Lihue, HI
- (Oral, Invited) Rencontres des Chimistes Théoriciens Francophones (RCTF2016), Lyon, France
- (Oral) 16<sup>th</sup> 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) 3<sup>rd</sup> International Conference on Chemical Bonding, Lihue, HI
- (Oral, invited) Symposium honoring Jack Simons’ 70<sup>th</sup> Birthday. Salt lake City, UT
- (Oral, invited) Symposium for the 43<sup>rd</sup> 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 – **Chosen as the Best Presentation of the session**
- (Oral, Invited) WATOC, Santiago, Chili
- (Oral) 2<sup>nd</sup> 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) 1<sup>st</sup> 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**) 3<sup>rd</sup> Molecular Materials Meeting (M3), Singapore

**2012:**

(Oral, invited) 7<sup>th</sup> Singapore International Chemistry Conference (SICC-7). Singapore  
(Oral, invited) Bridging the gap between ab initio and classical simulations, symposium at the 244<sup>th</sup> 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 70<sup>th</sup> Birthday, the 243<sup>th</sup> 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 70<sup>th</sup> 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. 234<sup>th</sup> 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. 20 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. 20<sup>th</sup> Symposium on Molecular Structure, Austin, TX, March **2004**.
- (Poster) Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H.-J.; Wang, L.-S. 225 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 Lectures**

### **2018:**

Molecular Foundry, nanoscience research facility at the Lawrence Berkeley National Laboratory  
Pennsylvania State University, Department of Chemistry  
John P. Reeves Distinguished Visiting Scientist Lectureship, Juniata College, Department of Chemistry

### **2017:**

Pittsburgh Quantum Institute, Women in Quantum Science & Engineering Lectureship

### **2016:**

Los Alamos National Laboratory, Division of Theory  
University of Colorado, Boulder, Department of Chemistry

Colorado State University, Department of Chemistry  
University of Texas in Austin, 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