

Anastassia N. Alexandrova

Curriculum Vitae

*Department of Chemistry and Biochemistry
University of California – Los Angeles
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Employment

- 2024-present** Charles W. Clifford Jr. Chair in Chemistry and Biochemistry
2022-present Professor. Department of Materials Science and Engineering, University of California, Los Angeles
2022-present Director of the NSF Center for Chemical Innovation, Advanced Molecular Architectures for Quantum Information Science
2019-present Professor. Department of Chemistry and Biochemistry, University of California, Los Angeles, and California NanoSystems Institute
2019-2022 Vice Chair for Undergraduate Education. Department of Chemistry and Biochemistry, University of California, Los Angeles
2015-2019 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. Department of Chemistry and Biochemistry, University of California, Los Angeles, 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. Alexander 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 State University, Russia.

Awards and Honors

- 2024** Quantum Bio-Inorganic Chemistry (QBIC) Prize – for groundbreaking research on the role of electrostatics in enzymatic catalysis
2024 Fellow of the Royal Society of Chemistry

2024	Royal Society of Chemistry Faraday Horizon Prize (given to the collaborative team: Anastassia N. Alexandrova, Hung-Chieh Cheng, Tao Cheng, Mengning Ding, Xiangfeng Duan, William A. Goddard III, Qiyuan He, Yu Huang, Zhihong Huang, Tianle Leng, Aamir Hassan Shah, Chengzhang Wan, Gongming Wang, Sibbo Wang, Zisheng Zhang, Guangyan Zhong), for Electrical transport spectroscopy (ETS) for experimentally determining Pt-surface hydronium pKa and local electrochemical environment
2020-2024	DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award (jointly with Philippe Sautet)
2023	UCLA Gold Shield Faculty Prize for academic excellence
2023	Brown Investigator Award by the Brown Science Foundation
2022	<i>Chemical Science</i> Reviewer Highlight Award
2022	Utah State University, Department of Chemistry and Biochemistry Alumni Achievement Award
2021	Max Planck-Humboldt Medal (jointly by the Max Planck Society and the Alexander von Humboldt Foundation, Germany)
2020	ACS PHYS Early Career Award in Theoretical Chemistry – for the development of theory of catalysis on dynamic heterogeneous interfaces based on statistical ensembles of metastable states, and applications particularly to surface-supported catalytic clusters.
2019	UCLA Distinguished Teaching Award for Senate Faculty
2018	Undergraduate Research Faculty Mentor Award, UCLA
2018	Cottrell Scholars Collaborative Academic Leadership Training Workshop
2016	Hanson-Dow Award for Excellence in Teaching, Department of Chemistry and Biochemistry, UCLA
2016	Herbert Newby McCoy Award for excellence in faculty research, Department of Chemistry and Biochemistry, UCLA
2016	Fulbright Scholarship from the U.S.-France Commission - <i>declined</i>
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	Kavli Fellow
2013	Alfred P. Sloan Research Fellowship
2011	Helman Fellowship, UCLA Faculty Career Development Award
2011	DARPA Young Faculty Award
2011	American Chemical Society YCC Leadership Development Award
2008	Mary Fieser Postdoctoral Fellowship at Harvard - <i>declined</i>
2008-2010	American Cancer Society Postdoctoral Fellowship
2005	Utah State University Robins Award: Graduate Research Assistant of the Year
2005	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
2005	USU School of Graduate Studies Dissertation Fellowship
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	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 research and academic achievements

Teaching

CHEM 249C, A Methods of Physical/Theoretical/Biophysical Chemistry; Methods of Materials Chemistry
 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
 CHEM 113B/213B, Methods of Quantum Chemistry

Course development, curriculum innovations, and integration of teaching and research:

CHEM 126/226, Computational Methods for Chemists (laboratory), development of the entirely new course, including the innovative final project that is a real research project done in the classroom. In 2012, 2013, 2020, and 2021 these resulted in publications with the students in the class.

CHEM 249 – students in class were given an assignment to work in groups of 3-6 to create thematic collections of papers from the ACS journals, and write introductory piece for the collection. One of these collections was accepted as the Virtual Special Issue in the *Journal of Physical Chemistry*, and was republished in all 4 parts of the journal, *JPC A*, *B*, *C*, and *Lett*.

Leadership in redesign and modernization of the theory and computation courses in the Department: CHEM 126/226, CHEM 125/225, and CHEM 245.

Professional Services

Campus and Departmental Services:

Theory and Computation graduate areal advisor (2015-present)
 Physical chemistry divisional Liasson (2023-present)
 Vice Chair for Undergraduate Education (2019-2022)
 Chemistry graduate advisor (2016-2019)
 General chemistry committee
 Graduate studies committee
 Curriculum committee
 IDRE advisory committee

Editorial Activities:

- 2024- Editorial Advisory Board, *J. Phys. Chem. Lett* (ACS)
- 2024- Board of Reviewing Editors (BoRE), *Science* magazine (AAAS)
- 2024- Editorial Advisory Board, *EES Catalysis* (RSC)
- 2023- Editorial Advisory Board, *ACS Catalysis* (ACS)
- 2023- Editorial Advisory Board, *Chemistry Europe* (Wiley)
- 2020- Senior Editor, *Journal of Physical Chemistry* (ACS)
- 2014-2016 Editor, *Scientific Reports* (Nature Publishing Group)
- 2014-2016 Editorial Advisory Board, *Journal of Physical Chemistry* (ACS)

Affiliations, National and International Services:

- Fellow of RSC
- Task group for IUPAC: revising the Gold book definitions of (anti)aromaticity concepts (2023-2024)
- Member of American Chemical Society
- Member of AAAS
- Chair of the Theory Subdivision of PHYS Division of the American Chemical Society (2015-2018)
- Member of WATOC
- DOE Basic Research Needs (BRN) service, Catalysis Section. 2017

Reviewing and review panel services:

- NSF, PRF, DOE, NIH, AFOSR, ERC (Europe)
- Pacific Northwest National Laboratory, “Molecular Theory and Modeling” program reviewer, 2023
- Periodic Review Board (PRB) service at Molecular Foundry, LBL, 2022
- Argonne National Laboratory, “Catalysis” program reviewer, 2021

Organizing and running scientific meetings:

- 2013-present** International Conference on Chemical Bonding (ICCB), Lihue, HI, USA (with Prof. Alexander Boldyrev and Prof. Lai-Sheng Wang)
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)
- 2026** ICQC 2026 Program Advisory Committee, Berkeley, CA, USA
- 2025** “Chemical physics of quantum information science” symposium at March APS meeting (with Prof. Tyrel McQueen)
- 2024** BORAM XVIII meeting, University of California Los Angeles (under the leadership of Prof. Alexander Spokoyny)
- 2024** Session “Computational Catalysis” at the Congress of the International Society for Theoretical Chemical Physics (ISTCP), Qingdao, China (with Profs. Jun Li, Nuria Lopez, Sergey Kozlov)
- 2024** Winter School at the UCLA Institute for Pure and Applied Mathematics, “QIS for chemistry and chemistry for QIS” (with Prof. Eric Hudson and Dr. Richard Ross)
- 2023** SoCal TheoChem 6.0 Symposium, UCLA, Los Angeles, CA, USA (with Prof. Benjamin Schwartz)
- 2022** Opening Keynote Session of the Spring National ACS Meeting on the topic of Chemical Bonding for Quantum Information Science. San Diego, CA, USA
- 2021** “Advanced Functional Clusters and Nanostructured Materials” symposium at PacifiChem, Honolulu, HI, USA (with Profs. Atsushi Nakajima, (Keio University, Japan), Scott L. Anderson (University of Utah), and Fengqi Song (Nanjing University, China))

2018	Scientific Committee, Aromaticity 2018, Riviera Maya, Mexico
2018	“Materials in extreme environments” symposium at the National ACS Meeting, Boston, MA, USA (with Prof. Eva Zurek)
2018	17 th International Conference of Theoretical Aspects of Catalysis (ICTAC), Los Angeles, CA (with Prof. Philippe Sautet)
2018	Advisory Board member of the Latin American Conference on Chemical Bonding, Brazil
2018	“Supported sub-nano clusters as the smallest and highly tunable interface for chemistry” symposium at the American Physical Society meeting, Los Angeles, CA (with Prof. Michael White)
2014	“Clusters in Catalysis” Symposium at the National ACS Meeting, Dallas, TX, USA (with Prof. Mark Saeys)
2013	“Chemistry in Silico” session 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	“Quantum Mechanics and Molecular Dynamics of Chemical and Biological Reactivity” meeting, satellite to the International Congresses of Quantum Chemistry, Los Angeles, CA, USA (with Prof. Houk)
2004	Abstract management and web-design for the Regional ACS Meeting of the Northwest / Rocky Mountains Sections, Logan, UT, USA

Presentations at Professional Meetings

2026:

(Oral, Invited) ICQC 2026, Berkeley, CA, USA

2025:

(Oral, Invited) MRS, Boston, MA, USA

(Oral, Invited) International Society of Electrochemistry Meeting, Mainz, Germany

(Honorary) QBIC Society meeting, Berlin, Germany

(Oral, Invited) Spring Annual Meeting of the Chemical Society of Japan, Osaka, Japan

(Oral, Invited) WATOC, Oslo, Norway

(Oral, contributed) APS March meeting, session "Advances in modeling chemical dynamics at molecule-metal interfaces", Anaheim, CA, USA

2024:

(Oral, Invited) Boron in the Americas (BORAM) XVIII, Los Angeles, CA

(Oral, Invited) Congress of the International Society for Theoretical Chemical Physics (ISTCP), Qingdao, China.

(Oral, Invited) Cold and Controlled Molecules & Ions (CCMI) conference, Institute of Science and Technology (ISTA), Austria

(**Key Lecture**) 17th International Conference on Theoretical Aspects of Catalysis (ICTAC), Seville, Spain.

(Oral, Invited) Molecular Interactions and Dynamics Gordon Research Conference, Stonehill College, Easton, Massachusetts

(Oral, Invited) American Conference on Theoretical Chemistry (ACTC), Chapel Hill, NC, USA.

(Oral, Invited) CECAM: Advances in catalytic reactivity simulations under operando conditions, Genova, Italy

(**Plenary**) Netherlands' Catalysis and Chemistry Conference (N3C), Noordwijkerhout, Netherlands

(Oral, Invited) 2024 Brown Institute for Basic Sciences Annual Meeting, Pasadena, CA, USA

(Oral, Invited) Molecular and atomic clusters Gordon Research Conference, Ventura, CA, USA

2023:

(Oral, Invited) Kavli institute for Theoretical Physics, Exploration Conference, Santa Barbara, CA, USA

(Oral, Invited) The SUNCAT Center for Interface Science and Catalysis, Summer Institute on Catalysis

(Oral, Invited) Fall National ACS Meeting, Symposium honoring Joachim Sauer, San Francisco, CA, USA

(Oral) Fall National ACS Meeting, Symposium "Catalyst Dynamics of Active Sites, Catalyst Structure, and Reaction Environment", San Francisco, CA, USA

(Oral, Contributed) 8th International Conference on Chemical Bonding, Kauai, HI, USA

(Oral, Invited) Nano Today Conference, San Diego, CA, USA

(Oral, Invited) Virtual Winter School on Theoretical Chemistry. Lectures and tutorials. With Prof. Mark Eberhart (Colorado School of Mines).

2022:

(Oral, Invited) XIII International Conference of the Russian-American Science Association (RASA), Los Angeles, CA

(Oral, Invited) Max Planck-Humboldt Symposium, Berlin, Germany

(Oral, Invited) ITAMP Workshop on Laser Cooling of Molecules, Cambridge, MA

(Oral, Invited, **Competitive**) Vistas in Catalysis - Chemical Sciences Roundtable at the National Academy of Science

(Oral, Invited) SoCal TheoChem, Riverside, CA

(Oral, Invited) Pacific Coast Catalysis Society meeting, Riverside, CA

(**Oral, Distinguished Lectureship**) 3rd European Symposium on Chemical Bonding: "CBOND2022 Amsterdam online"

(Oral) 7th International Conference on Chemical Bonding, Kauai, HI, USA

(Oral, Invited) Gordon Research Conference, Atomically precise nanochemistry, Ventura, CA, USA

(**Oral, Keynote**) 16th International Conference on Theoretical Aspects of Catalysis, Lyon, France

(Oral, Invited) Gordon Research Conference, Catalysis. New London, NH, USA

(**Oral, Keynote**) Spring National ACS Meeting, Symposium "Bridging Surface Science to Catalysis", San Diego, CA, USA

(**Oral, Keynote**) Opening Keynote Session of the Spring National ACS Meeting, San Diego, CA, USA

2021:

- (Oral, Invited) PacifiChem, Honolulu, HI, Symposium “Advanced Functional Clusters and Nanostructured Materials”
- (Oral, Invited) Pacific Coast Catalysis Society Meeting (virtual)
- (Oral, Invited) Quantum Bio-Inorganic Chemistry Society (QbtopIC) lecture series, Groningen, Netherlands
- (Oral, Invited) Symposium on size-selected clusters, Prague, Czech Republic
- (Oral, Invited) SUNCAT panel on Metal Nanoparticle Catalysis
- (Oral, Invited) Spring virtual National ACS Meeting, Symposium “Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization, and Performance Studies”
- (Oral, Invited) Humboldt-Plank Symposium, Germany

2020:

- (Oral, Invited) Fall ACS Meeting, ACS Physical Chemistry Award Symposium
- (Oral, Invited) Spring ACS Meeting, Symposium “Elucidation of Mechanisms & Kinetics on Surfaces”, Philadelphia, PA, USA *–canceled due to pandemics*
- (**Keynote**) Spring ACS Meeting, Symposium “Bringing Surface Science to Catalysis”, Philadelphia, PA, USA *–canceled due to pandemics*
- (**Keynote**) Spring ACS Meeting, Symposium “Activation of light (C1-C4) hydrocarbons. Theory & Experiments”, Philadelphia, PA, USA *–canceled due to pandemics*
- (Oral) Spring ACS Meeting, Symposium “Advances in Understanding Dynamic Structural Evolution During Catalysis using Experiment & Theory”, Philadelphia, PA, USA *–canceled due to pandemics*
- (Oral) Spring ACS Meeting, Symposium “Well-Defined Materials for Heterogeneous Catalysis: Synthesis, Characterization & Performance Studies”, Philadelphia, PA, USA *–canceled due to pandemics*
- (Oral) Spring ACS Meeting, Symposium “Computational design of artificial metalloenzymes through quantum mechanical and mixed quantum-classical approaches”, Philadelphia, PA, USA *–canceled due to pandemics*
- (Oral) #STEMToo Seminar and round table, San Diego State University, female students’ invited participant and mentor
- (**Plenary**) S3C - Symposium on Size-Selected Clusters, Davos, Switzerland

2019:

- (Oral, Invited) Fall National ACS Meeting, Symposium dedicated to the 75th Birthday of Prof. Henry F. Schaefer III, San Diego, CA
- (Oral, Invited) Fall National ACS Meeting, Symposium “Amorphous Materials: Challenges and Opportunities”, San Diego, CA
- (Oral, Invited) Fall National ACS Meeting, Symposium and mentorship event “Women make COMP”, San Diego, CA
- (**Plenary**) 18th International Conference on Density Functional Theory and its Applications, Alicante, Spain
- (Oral, Invited) Catalytic Reactivity in Complex Environments Workshop, Pacific Northwest National Laboratory, Richland, WA

(**Plenary**) 7th Annual OpenMolcas Developers' Workshop, Minneapolis, MN

(**Keynote**) The 4th Symposium of the Chinese Computational Catalysis Network (C3N-4), Xi'an, China

(Oral, Invited) Spring National ACS Meeting, Symposium "Model Catalysis: Materials Complexity Frontiers", Orlando, FL

(Oral, Invited) Spring National ACS Meeting, Symposium "Advances in Selective Oxidation Catalysis" in honor to the recipient of the 2019 National *Ipatieff Prize*, Ive Hermans, Orlando, FL

(Oral, Invited) Spring National ACS Meeting, Symposium "Through the Lens of Inorganic Chemistry: Understanding Heterogeneous Processes in Energy Conversion and Storage", Orlando, FL

2018:

(Oral, Invited) Aromaticity 2018, Riviera Maya, Yucatan, Mexico

(**Plenary**) European Symposium on Chemical Bonding, Oviedo, Spain

(Oral, Invited) Fall National ACS Meeting, Symposium "Understanding Catalytic Sites on Amorphous and Disordered Materials", Boston, MA

(Oral) 6th International Conference on Chemical Bonding, Lihue, HI

(Oral, Invited) International Congress of Quantum Chemistry (ICQC), Menton, 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) 5th 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) 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 – **Chosen as the Best Presentation of the session**
- (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 (IQTUB), 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. 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. 20th 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**.

Invited Lectures

2025:

University of Pennsylvania, **Trustees' Council of Penn Women Lecture in Chemistry**
Tokyo Institute of Technology
University of Minnesota, Department of Chemistry
Washington State University, Department of Chemistry

2024:

Shell, Chemistry and Catalysis Webinar
University of Texas, Austin, Department of Materials Science
Northwestern University, Department of Chemistry and Biochemistry
University of Oregon, Department of Chemistry, **student-invited colloquium speaker**
University of Science and Technology of China, Department of Theoretical Chemistry, Hefei, China
University of Science and Technology of China, School of Chemistry, Hefei, China, **honorary Jingzhi lecture series**
Naval Research Laboratory, **distinguished speaker**
Saratov University, Department of Chemistry, Russia (virtual)
Tianjin University, China, **distinguished lectureship** (virtual)

2023:

University of Vermont, Department of Chemistry
Brandeis University, Department of Chemistry
Washington University in St. Louis, Department of Chemistry
University of California, Berkeley, Department of Chemistry
Ohio State University, Department of Chemistry

2022:

University of Arizona, Department of Chemistry
University of California, Irvine, Department of Materials Science and Engineering
Columbia University, Department of Chemistry
TU Delft, Netherlands. Delft Catalysis Days seminar series.
Fritz-Haber Institute of the Max Planck Society, Berlin, Germany

Utah State University, Department of Chemistry and Biochemistry
California State University, Long Beach, Department of Chemistry
NSF Center for Integrated Catalysis (CIC), UCLA
Boston College, Department of Chemistry
University of California, Los Angeles, Department of Materials Science and Engineering

2021:

Institut de Química Teòrica i Computacional (IQTUB), Universitat de Barcelona, Spain
University of Houston, Department of Chemistry
University of Illinois, Urbana-Champaign, Department of Chemistry
University of South Carolina, Department of Chemical Engineering
The 5 collaborative catalysis consortia across Germany; talk hosted by Das Institut für Katalyseforschung und Technologie (IKFT)
Geffen Academy at UCLA (middle and high school), UCLA Day at Geffen
Highlands in Chemistry seminar, Virginia Tech University, Department of Chemistry

2020:

Iowa State University, Department of Chemistry
University of Oregon, Department of Chemistry
Claremont Colleges (Harvey Mudd, Pomona, Scripps, Pitzer, Claremont McKenna)
Universidad de Chile, Santiago, Chile, Departamento de Física

2019:

MIT, Department of Chemistry
Woodward Colloquium, Harvard University, Department of Chemistry and Chemical Biology
Rutgers University, Department of Chemistry
University of Utah, Department of Chemistry
University of California Davis, Department of Chemistry
University of California Santa Barbara, Department of Chemistry
George Washington University, Department of Chemistry
University of Tennessee, Department of Chemistry

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 (a series of research lectures of increasing difficulty, targeting undergraduate student audiences)

2017:

Women in Quantum Science & Engineering Lectureship, Pittsburgh Quantum Institute

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 Islands, 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