

# 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
- 2019-present** Professor. Department of Chemistry and Biochemistry, University of California, Los Angeles, and California NanoSystems Institute
- 2022-2025** Director of the NSF Center for Chemical Innovation, Advanced Molecular Architectures for Quantum Information Science
- 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

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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. 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.

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### Awards and Honors

- 2026** Foreign Visitor Program at ICASEC - International Center for Advanced Studies of Energy Conversion, Göttingen, Germany

- 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, Sibowang, 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 *Chemical Science* 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 - *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 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 - *declined*
- 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 (*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 research and academic achievements
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## **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.

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## **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 “The emergence of topological catalysis” symposium at the Spring National ACS Meeting, Atlanta, GA, USA (with Prof. Andrew Rappe)
- 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<sup>th</sup> 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. 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 “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
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## **Presentations at Professional Meetings**

### **2026:**

- (Oral, Invited) ICQC 2026, Berkeley, CA, USA
- (Oral, Invited) Fall National ACS Meeting, symposium “Treatment of Electrostatics and Polarization in the Simulation of Materials, Biomolecules, and Interfaces”, Chicago, IL, USA
- (Oral, contributed) Faraday Discussions, London, UK
- (Oral, Invited) Symposium on Size-Selected Clusters, Davos, Switzerland
- (Keynote Lecture)** Spring National ACS Meeting, symposium "Catalysis under External Stimuli: From Design to Dynamic Control in Homogeneous and Heterogeneous Systems", Atlanta, GA, USA
- (Oral, Invited) Spring National ACS Meeting, symposium “Kinetic and Mechanistic Insights to Catalysis”, Atlanta, GA, USA
- (Oral, contributed) Spring National ACS Meeting, symposium “The emergence of topological catalysis”, Atlanta, GA, USA

### **2025:**

- (Oral, Invited) 2025 SSRL/LCLS Users' Meeting, Palo Alto, CA, USA
- (Oral, Invited) International Society of Electrochemistry Meeting, Mainz, Germany
- (Honorary)** QBIC Society meeting, Berlin, Germany
- (Oral, contributed) International Conference on Chemical Bonding, Kauai, HI, USA

(Oral, Invited) National ACS Meeting, symposium honoring Dr. Simon Bare for extraordinary achievements in the field of catalysis, Washington DC, USA  
(Oral, Invited) Inaugural Meeting of the Rudolph A. Marcus Center for Theoretical Chemistry, Caltech, Pasadena, CA, USA  
(Oral, Invited) WATOC, Oslo, Norway  
(Oral, Invited) 2025 Brown Institute for Basic Sciences Annual Meeting, Pasadena, CA, USA  
(Oral, Invited) USC Stauffer symposium, Los Angeles, CA, USA  
(Oral, contributed) APS March meeting, session "Advances in modeling chemical dynamics at molecule-metal interfaces", Anaheim, CA, USA  
(Oral, Invited) Spring Annual Meeting of the Chemical Society of Japan, Osaka, Japan

#### 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**) 17<sup>th</sup> 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) 8<sup>th</sup> 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**) 3<sup>rd</sup> European Symposium on Chemical Bonding: "CBOND2022 Amsterdam online"

- (Oral) 7<sup>th</sup> International Conference on Chemical Bonding, Kauai, HI, USA
- (Oral, Invited) Gordon Research Conference, Atomically precise nanochemistry, Ventura, CA, USA
- (Oral, Keynote)** 16<sup>th</sup> 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 75<sup>th</sup> 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)** 18<sup>th</sup> 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) 6<sup>th</sup> 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) 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 (IQTUCUB), 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. 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**.
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## **Invited Lectures**

### **2026:**

University of Chicago, Department of Chemistry  
Princeton University, Department of Chemistry

### **2025:**

Washington State University, Department of Chemistry  
University of Minnesota, Department of Physics  
Yale University, Department of Chemistry  
University of California, Berkeley, Department of Materials Science and Engineering, **Graduate Student Invited Seminar**  
University of Pennsylvania, **Trustees' Council of Penn Women Lecture in Chemistry**  
Tokyo Institute of Technology

### **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 (IQTCUB), 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 Katalysforschung 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 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