

## Curriculum Vitae

**SOTIRIS S. XANTHEAS**

3501 Equestrian Dr. West Richland, WA, 99353 USA Tel. (509) 438-0512 <a href="mailto:xeffie@aol.com">xeffie@aol.com</a>	Advanced Computing, Mathematics & Data Pacific Northwest National Laboratory 902 Battelle Boulevard, P.O. Box 999, MS J7-10, Richland, WA 99352 Tel. (509) 375-3684 <a href="mailto:sotiris.xantheas@pnnl.gov">sotiris.xantheas@pnnl.gov</a>	Affiliate Professor UW-PNNL Distinguished Faculty Fellow Department of Chemistry, University of Washington, Seattle, WA 98195 <a href="mailto:xantheas@uw.edu">xantheas@uw.edu</a>
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**Education**

August 1984 – September 1990	Iowa State University, Ames, Iowa, USA <i>Advisor:</i> Prof. Klaus Ruedenberg Ph.D. granted May 1991 <i>Major:</i> Physical Chemistry <i>Minor:</i> Solid State Physics
September 1979 – June 1984	National Technical University of Athens, GREECE Diploma in Chemical Engineering granted June 1984 <i>Major:</i> Chemical Engineering

**Professional Employment**

January 2022 – present	<b>Director, Computational &amp; Theoretical Chemistry Institute (CTCI) at PNNL</b>
June 2004 – present	<b>Laboratory Fellow</b>
January 1998 – May 2004	<b>Chief Scientist</b>
April 1993 – December 1997	<b>Senior Research Scientist</b>
August 1992 – March 1993	<b>Research Scientist</b> Pacific Northwest National Laboratory Richland, Washington USA
September 1990 – July 1992	<b>Postdoctoral Fellow</b> Molecular Science Research Center Pacific Northwest Laboratory Richland, Washington USA <i>Research advisor:</i> Thomas H. Dunning, Jr.
June 1985 – August 1990	<b>Research Associate</b> Ames Laboratory, US Department of Energy Ames, Iowa USA
August 1984 – June 1985	<b>Teaching Assistant</b> Department of Chemistry Iowa State University, Ames, Iowa USA
January 1984 – June 1984	<b>Research Fellow</b> Institute for Inorganic & Analytical Chemistry

University of Innsbruck, AUSTRIA  
 Research advisor: Prof. Bernd M. Rode

### Personal information

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Born 20 June 1961 in Athens, Greece. Greek citizen, US permanent resident  
 Married, two daughters

### Citation Index

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Web of Knowledge:	Total of 14,728 citations (as of March 25 <sup>th</sup> , 2025)	Hirsch index: 67
Google Scholar:	Total of 19,308 citations (as of March 25 <sup>th</sup> , 2025)	Hirsch index: 74

### University Affiliations

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*Gauss Professor*, University of Göttingen, Göttingen, Germany (2022)  
*Specially Appointed Professor*, World Research Hub Initiative, Tokyo Institute of Technology, Tokyo, Japan (2019 – 2025)  
*Affiliate Professor*, *UW-PNNL Distinguished Faculty Fellow*, Department of Chemistry, University of Washington, Seattle, WA, USA (September 2016 – present)  
*Adjunct Professor*, Department of Mathematics, Washington State University, Pullman, WA, USA (December 2014 – present)  
*Visiting Professor*, Department of Physics, Technical University of Munich, Garching, Germany (June – July 2009)  
*Visiting Professor*, Department of Chemistry, University of Kaiserslautern, Kaiserslautern, Germany (September 2003 – May 2004)  
*Affiliated Scientist*, Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, Heraklion, Crete, Greece (1996 – present)  
*Instructor*, Physical Chemistry, Department of Chemistry, Iowa State University, Ames, Iowa, USA: Fall Semester 1987 (Thermodynamics), Fall Semester 1988 (Quantum Mechanics)

### Fellowships

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Northwest College and University Association for Science Fellow, 1990 – 92  
 Austrian Federal Ministry for Science and Research Fellow, 1984

### Awards and Distinctions – Professional Recognition

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*Morino Lecture*, The Morino Foundation for Molecular Science, Tokyo, Japan, March 2026  
*Renewed Research Stay* at the University of Bochum, Germany, Alexander von Humboldt Foundation, March 2026  
*Director*, Computational and Theoretical Chemistry Institute (CTCI) at PNNL (2022 – present)  
*Appointed Gauss Professor*, Göttingen Academy of Sciences, Göttingen, Germany (2022)  
*Elected member*, *Board of Regents*, University of Peloponnese, Greece (2022)  
*ICASEC Fellow*, International Center for Advanced Studies of Energy Conversion, University of Göttingen, Göttingen, Germany (2022)  
*Elected Member*, Washington State Academy of Sciences (WSAS), July 2018

Citation: "For fundamental contributions to the understanding of molecular interactions and collective phenomena in aqueous systems"

*Fulbright Scholar*, Institute for International Education, Department of Molecular Biology and Genetics, Democritus University of Thrace, Greece (September – October 2017)

*Renewed Research Stay* at the University of Göttingen, Germany, Alexander von Humboldt Foundation, July 2015

*Editorial Advisory Board*, The Journal of Chemical Physics (January 2015 – December 2017)

*Director's Award for Exceptional Scientific Achievement* (1 award annually), Pacific Northwest National Laboratory (June 2013)

*Advisory Editorial Board Member*, Chemical Physics Letters (January 2013 – December 2015); *Renewed* (January 2016 – December 2018).

*Visiting Fellow*, Institute for Advanced Study, Technical University of Munich, Germany (August – September 2012)

*Editorial Advisory Board (EAB) Member*, The Journal of Physical Chemistry (January 2012 – December 2014)

*Fellow*, Japan Society for the Promotion of Science (JSPS), March 2011

*Science and Technology Achievement Recognition (STAR) award*, Pacific Northwest National Laboratory, February 2010

*Fellow*, American Association for the Advancement of Science (AAAS), February 2010

Citation: "For fundamental contributions to the understanding of molecular interactions in aqueous systems"

*Henry Eyring Lecture*, Department of Chemistry, University of Utah, Salt Lake City, Utah, April 2009

*Renewed Research Stay* at the Technical University of Munich at Garching, Germany, Alexander von Humboldt Foundation, February 2009

*Science and Technology Achievement Recognition (STAR) award*, Pacific Northwest National Laboratory, January 2008

*Outstanding Performance Award*, Fundamental and Computational Sciences Directorate, Pacific Northwest National Laboratory, October 2007

*Marie Curie Fellow*, Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, Heraklion, Greece, July 2007

*Fellow*, American Physical Society (APS), November 2005

Citation: "For fundamental contributions to the understanding of molecular interactions in aqueous systems"

*Laboratory Fellow*, Pacific Northwest National Laboratory's highest rank (top 1%) for scientific and professional staff, June 2004

*Outstanding Performance Award for Outstanding Project Research – DOE Basic Energy Sciences*, Fundamental Science Directorate and Energy Science and Technology Directorate, Pacific Northwest National Laboratory, 2004

*Outstanding Performance Award*, Fundamental Science Directorate, Pacific Northwest National Laboratory, 2003

*Director's Award for Outstanding Performance*, Pacific Northwest National Laboratory, 2003

*Friedrich Wilhelm Bessel Research Award*, Alexander von Humboldt Foundation, 2003

*Outstanding Teaching Assistant Award*, Department of Chemistry, Iowa State University, 1990

*All University Teaching Excellence Award*, Iowa State University, 1990

*Award for Excellence in Graduate Research*, Alpha Chi Sigma Chapter of the American Chemical Society, Iowa State University, 1990

*G. Stathis Memorial Award* administered by the University of Chicago, 1988

### Other Activities

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*Editorial Board:* International Journal of Molecular Sciences (IJMS), Section: Physical Chemistry and Chemical Physics (2018 – present)

*Reviewer:* *Agencies:* The National Science Foundation (US), US Department of Energy (Office of Basic Energy Sciences), NATO (Scientific Affairs Division), The Petroleum Research Fund, European Research Council, Australian Research Council, The Israel Science Foundation, Kentucky Science and Engineering Foundation, Research Corporation (Canada), Czech Science Foundation, European Research Council (ERC)

*Journals:* Nature, Science, Angewandte Chemie, Proceedings of the National Academy of Sciences (USA), Chemical Reviews, The Journal of the American Chemical Society, Physical Review Letters, The Journal of Physical Chemistry, The Journal of Chemical Physics, Theoretica Chimica Acta, Comptes Rendus de l' Académie des Sciences Série IIc - Chimie, Molecular Physics, Chemical Physics Letters, Theochem, International Journal of Mass Spectrometry and Ion Processes, Chemical Physics, Physical Chemistry Chemical Physics, International Journal of Quantum Chemistry, Journal of Raman Spectroscopy, Theoretical Chemistry Accounts, Journal of Computational Chemistry, Journal of Cluster Science, Journal of Molecular Liquids, Spectrochimica Acta A, Geochimica et Cosmochimica Acta, Inorganic Chemistry, Journal of Polymer Science B, Philosophical Magazine Letters, Journal of Chemical Theory and Computation, Canadian Journal of Chemistry, Journal of Physical Chemistry Letters, Journal of Biophotonics, Dalton Transactions, International Journal of High Performance Computing, Journal of Integrative Environmental Sciences, Molecular Biosystems, ChemComm, Journal of Materials Science, New Journal of Chemistry, Zeitschrift für Physikalische Chemie, International Journal of Hydrogen, Wiley Interdisciplinary Reviews, Computational & Theoretical Chemistry, ChemSusChem, European Physical Journal D, Analytica Chimica Acta, Molecular Simulation, The Biophysical Journal, Accounts of Chemical Research, ChemPhysChem, Thermochemica Acta, Scientific Reports, Nanoscale, Chemical Science, ACS Omega, Journal of the American Society for Mass Spectrometry

*Assessor,* Australian Research Council

*Manager,* Supercomputer allocations at the National Energy Research Supercomputer Center (Berkeley, CA) for the Molecular Theory Group, Environmental Molecular Sciences Laboratory (1992 – present)

*Research Advisor*

*Postdoctoral Fellows:* CJ Burnham, GS Fanourgakis, S Yoo, T Yoshida, E Miliordos, J Mato (PNNL), J Warneke (PNNL, Feodor-Lynen Fellow from the Alexander von Humboldt Foundation), HE Dorsett (joint with Univ. of Melbourne, Australia)

*Graduate students:* ER Batista (joint with Univ. of Washington), GS Fanourgakis (joint with Univ. of Crete, Greece), D Tzeli (joint with Univ. of Athens, Greece), C Kefalidis (joint with Univ. of Thessaloniki, Greece), A Lagutschenkova (joint with Univ. of Kaiserslautern, Germany), JC Werhahn (joint with Technical Univ. of Munich, Germany), D Akase (joint with Hiroshima Univ., Japan), JP Heindel, KM Herman, GD Santis, MP Hoffman, MN Hallsten, R Irving, A Hale, L Ngyuen (Univ. of Washington)

### Membership in Professional Societies

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American Chemical Society (ACS)  
American Physical Society (APS) – Fellow (2005)  
American Association for the Advancement of Science (AAAS) – Fellow (2010)

### Internal Committee Assignments

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- Initiative Lead*, Open Call Laboratory Directed Research & Development (LDRD) program, Pacific Northwest National Laboratory (2016 – present). Responsible for the award and management of \$1.8M per year in internal funds
- Member*, Linus Pauling Distinguished Postdoctoral Fellowship Selection Committee, Pacific Northwest National Laboratory (2012 – present)
- Member*, Open Call Laboratory Directed Research and Development (LDRD) Committee (2012 – 2015)
- Elected Member*, Executive Committee, Council of Fellows, Pacific Northwest National Laboratory (2009 – present)
- Member*, Advisory Committee on Extreme Scale Computing Initiative, Pacific Northwest National Laboratory (2008 – 2013)
- Member*, Advisory Committee, High Performance Computational Chemistry-2 hardware upgrade, Molecular Science Computing Facility, Environmental Molecular Sciences Laboratory (2001)
- Chairman*, National Energy Research Supercomputer Center (NERSC) subcommittee, Environmental Molecular Sciences Laboratory (1993 – 1996)
- Member*, Computer Resources Committee (CRC), Environmental Molecular Sciences Laboratory (1993 – 1996)

### External Committee Assignments

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- Reviewer*, Chemical Physics Program at Sandia National Laboratory (SNL) for the US Department of Energy, Office of Basic Energy Sciences, Biosciences and Geosciences, Livermore, CA, USA (June 24 – 26, 2020)
- Invited Panelist*, NSF / Chemistry panel on Quantum Chemistry (CTMC Quantum Chemistry), Washington DC, USA (January 13 - 14, 2020)
- Invited Panelist*, NSF / Chemistry panel on Quantum Chemistry (CTMC Quantum Chemistry 2), Washington DC, USA (February 13, 2017)
- Invited Panelist*, NSF / Chemistry panel on Quantum Dynamics and Spectroscopy (CTMC Model Development), Washington DC, USA (February 4, 2016)
- Invited Tutorial* “Hofmeister Effect and Ion Recognition” presented at the NSF workshop on “*Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions*”, Washington, DC, USA (May 31 – June 4, 2015)
- Reviewer*, Chemical Physics Program at Lawrence Berkeley National Laboratory (LBNL) for the US Department of Energy, Office of Basic Energy Sciences, Biosciences and Geosciences, Berkeley, CA, USA (May 12 – 15, 2015)
- Invited Panelist*, NSF / Chemistry panel on Quantum Dynamics and Spectroscopy (CTMC QDYNESPEC), Washington DC, USA (February 18, 2015)
- Invited Lecturer*, NSF workshop on the Conceptualization of a Molecular Computation Software Institute, Houston, TX, USA (January 22 – 24, 2015)
- Invited Lecturer*, workshop on Fundamental Challenges in our Understanding of the Physics and Chemistry of Water, University of Houston, Houston, TX, USA (January 16 – 17, 2015)
- Member, Jury Committee*, selection of the new Fellows for the Advanced Study Institute of the Technical University of Munich (IAS – TUM), Garching, Germany (June 2014)

- Invited Panelist*, Program Requirement Review "*Large Scale Production Computing and Storage Requirements for Basic Energy Sciences*", Office of Basic Energy Sciences (BES) & Office of Advanced Scientific Computing Research (ASCR), U.S. Department of Energy and the National Energy Research Scientific Computing Center (NERSC), Gaithersburg, MD, USA (October 8 – 9, 2013)
- Panelist*, Workshop on "*Computational Materials Science and Chemistry for Innovation*", Bethesda, MD, USA (July 2010)
- Member*, Executive committee, American Chemical Society (ACS), Division of Physical Chemistry, 2009 – 2012
- Member*, Review Panel, Chemical Sciences, Geosciences and Biosciences Division, US Department of Energy (April 2009)
- Member*, Committee of Visitors in Atomic, Molecular and Optical Sciences and Gas-Phase Chemical Physics Programs for the Chemical Sciences, Geosciences and Biosciences Division of the Basic Energy Sciences, US Department of Energy (April 2008)
- Member*, Panel on "Opportunities for Catalysis Science in the 21<sup>st</sup> Century", US DoE, Gaithersburg, Maryland (May 2002)
- Member*, Evaluation Committee for the Graduate Program, Department of Chemistry, University of Crete, Greece (July 1999)
- Member*, Review Panel "Carbon Management Initiative and Complex Phenomena Program", US DoE, Washington DC (May 1999)
- Member*, Evaluation Committee for the Undergraduate Program, Department of Chemistry, University of Crete, Greece (September 1998)

#### **Invited Lectures at Scientific Institutions**

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- 1987 Institute for Inorganic & Analytical Chemistry, University of Innsbruck, Austria (January)
- 1987 Iowa State University, Ames, Iowa, USA; Physical Chemistry Seminar, (November)
- 1987 Michigan State University, East Lansing, Michigan, USA; Physical Chemistry Seminar (November)
- 1988 Institute for Electronic Structure and Laser, University of Crete, Heraklion, Greece; Departmental Seminar (August)
- 1990 Pacific Northwest Laboratory, Richland, Washington, USA (January)
- 1990 Exxon Research and Engineering, Clinton, New Jersey, USA (February)
- 1990 National Hellenic Research Foundation, Athens, Greece (July)
- 1992 Ames Laboratory, U. S. Department of Energy, Ames, Iowa, USA (December)
- 1994 Daresbury Laboratory, Cheshire, United Kingdom (June)
- 1994 Mansfield College, University of Oxford, Oxford, United Kingdom (July)
- 1995 University of California, Berkeley, CA, USA; Physical Chemistry Seminar (March)
- 1995 University of Washington, Seattle, WA, USA; Physical Chemistry Colloquium (May)
- 1995 Foundation for Research and Technology-Hellas, Heraklion, Greece (July)
- 1996 Technical University of Munich at Garching, Germany; Physical Chemistry Seminar (May)
- 1996 Theoretical Chemistry Division, University of Innsbruck, Austria (May)
- 1996 New York University, New York, NY USA; Physical Chemistry Seminar (June)
- 1996 Daresbury Laboratory, Engineering and Physical Sciences Research Council, UK (October)
- 1997 University of Crete, Greece; Advanced Physics Summer School, Heraklion, Greece (July)
- 1999 University of Colorado, Boulder, Colorado, USA; Physical Chemistry Colloquium (February)
- 1999 Colorado State University, Fort Collins, Colorado, USA; Physical Chemistry Colloquium (February)
- 1999 University of California, Berkeley, CA, USA; Department of Chemistry Special Seminar (March)
- 1999 Department of Applied Chemistry, University of Tokyo, Tokyo, Japan; Joint Tokyo Theoretical Chemistry Seminar (March)
- 1999 Tokyo Metropolitan University, Tokyo, Japan; Chemistry Department Seminar (December)

- 2000 Columbia University, New York, New York, USA; Department of Chemistry & Center for Biomolecular Simulation Seminar Series (February)
- 2000 Emory University, Atlanta, Georgia, USA; Physical Chemistry Colloquium (March)
- 2000 University of Georgia, Athens, Georgia, USA; Physical Chemistry Colloquium (March)
- 2000 Hebrew University of Jerusalem and Fritz Haber Center for Molecular Dynamics Research, Jerusalem, Israel; Departmental Seminar (April)
- 2000 Sandia National Laboratories, Albuquerque, New Mexico, USA; Physics and Chemistry Colloquium Series (October)
- 2001 University of North Carolina, Chapel Hill, North Carolina, USA; Physical Chemistry Colloquium (February)
- 2001 Iowa State University, Ames, Iowa, USA; Physical Chemistry Colloquium (February)
- 2001 New York University, New York, New York, USA; Chemistry Department Seminar (December)
- 2002 University of Ioannina, Ioannina, Greece; Chemistry Department Seminar (September)
- 2002 Institute for Physical and Theoretical Chemistry, Technical University of Munich, Garching, Germany; Departmental Seminar (September)
- 2002 University of Kaiserslautern, Kaiserslautern, Germany; Chemistry Department Seminar (September)
- 2002 Institute for Physical and Theoretical Chemistry, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany; Departmental Seminar (September)
- 2003 California Institute of Technology, Pasadena, California, USA; Chemical Physics Seminar Series (May)
- 2003 University of Western Ontario, London, Ontario, Canada; Physical Chemistry Colloquium (November)
- 2003 Institute for Physical and Theoretical Chemistry, Technical University of Munich, Garching, Germany; Institute Colloquium (December)
- 2003 Aristotle University of Thessaloniki, Thessaloniki, Greece; Chemistry Department Seminar (December)
- 2004 Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany; Institute Colloquium (January)
- 2004 Oxford University, Oxford, United Kingdom; Theoretical Chemistry Colloquium (February)
- 2004 Cambridge University Chemical Laboratory, Cambridge, United Kingdom; Theoretical Chemistry Colloquium (February)
- 2004 Christian-Albrechts University, Kiel, Germany; Gesellschaft Deutscher Chemiker (GDCh) Colloquium Series, Department of Chemistry (April)
- 2004 University of Würzburg, Würzburg, Germany; Gesellschaft Deutscher Chemiker (GDCh) Colloquium Series, Institute for Physical Chemistry (May)
- 2004 Max-Planck-Institute für Kohlenforschung, Mülheim an der Ruhr, Germany, Seminar Series (June)
- 2004 University of Delaware, Newark, Delaware, USA; Physical/Analytical Chemistry Colloquium (November)
- 2006 University of Nebraska-Lincoln, Lincoln, Nebraska, USA; Department of Chemistry Colloquium (March)
- 2006 Technical University of Kaiserslautern, Kaiserslautern, Germany; Department of Chemistry Colloquium (May)
- 2006 Ruhr-Universität Bochum, Bochum, Germany; Physical Chemistry Seminar (July)
- 2006 University of Wisconsin, Madison, Wisconsin, USA; Physical Chemistry Seminar (September)
- 2007 Kyoto University, Katsura Campus, Kyoto, Japan; Physical Chemistry Seminar (March)
- 2007 Hiroshima University, Hiroshima, Japan; Physical Chemistry Seminar (March)
- 2007 Institute for Molecular Structure, Okazaki, Japan; Theoretical Division Seminar (March)
- 2007 Waseda University, Tokyo, Japan; Physical Chemistry Seminar (March)
- 2007 Boston University, Boston, Massachusetts, USA; Chemistry Colloquium (September)

- 2007 Massachusetts Institute of Technology, Cambridge, Massachusetts, USA; Greater Boston Area (Harvard University, Massachusetts Institute of Technology, Boston University, Boston College) Theoretical Chemistry Lecture Series (September)
- 2007 Technical University of Munich, Department of Physics, Garching, Germany; Seminar (December)
- 2007 Leopold-Franzens University of Innsbruck, Institute of General, Inorganic and Theoretical Chemistry, Innsbruck, Austria; Theoretical Division Seminar (December)
- 2008 University of California, Davis, California, USA; Chemistry Department Seminar (February)
- 2009 Southern Illinois University, Carbondale, Illinois, USA; Department of Chemistry & Biochemistry Seminar (February)
- 2009 Rutherford Appleton Laboratory, Didcot, UK; ISIS Seminar Series (March)
- 2009 University of Utah, Salt Lake City, Utah, USA; Henry Eyring Lecture (April)
- 2009 Fritz Haber Institute of the Max Planck Society, Berlin, Germany; Department of Molecular Physics Seminar (June)
- 2009 Technical University of Munich at Garching, Garching, Germany; Department of Physics E11 Seminar (July)
- 2009 SLAC National Accelerator Laboratory, Palo Alto, CA, USA; Seminar (September)
- 2009 Argonne National Laboratory, Chemical Sciences & Engineering Division, Argonne, Illinois, USA; Chemical Sciences and Engineering Division Seminar (November)
- 2010 University of Illinois, Urbana-Champaign, Illinois, USA; Physical Chemistry Seminar (February)
- 2010 University of California San Diego, San Diego, CA, USA; Physical Chemistry Seminar (February)
- 2010 Technical University of Munich at Garching, Garching, Germany; Department of Physics E11 Seminar (May)
- 2010 University of Zurich, Zurich, Switzerland; Physical Chemistry Institute Seminar (June)
- 2010 Washington State University, Pullman, WA, USA; Department of Chemistry Seminar (October)
- 2010 Kasetsart University, Bangkok, Thailand; Department of Chemistry Seminar (November)
- 2011 University of Hiroshima, Hiroshima, Japan; Department of Chemistry Seminar (March)
- 2011 Institute for Molecular Structure, Okazaki, Japan; Theoretical Division Seminar (March)
- 2011 Tokyo Metropolitan University and Tokyo Technological University; joint Chemistry Colloquium (September)
- 2011 University of Nagoya, Nagoya, Japan; Department of Applied Chemistry Seminar (September)
- 2011 University of Western Ontario, London, Canada; Department of Chemistry Seminar (September)
- 2011 Photon Science Division, SLAC National Accelerator Laboratory, Menlo Park, CA; Department Seminar (November)
- 2012 Ohio State University, Columbus, Ohio, USA; Physical Chemistry Seminar (April)
- 2012 Ludwig Maximilian University (LMU), Munich, Germany; Theoretical Chemistry Seminar (September)
- 2012 Leopold-Franzens University of Innsbruck, Institute of General, Inorganic and Theoretical Chemistry, Innsbruck, Austria; Theoretical Division Seminar (September)
- 2012 Technical University of Munich, Garching, Germany; Physics E-11 Colloquium (September)
- 2012 University of Göttingen, Germany; Physical Chemistry Department Seminar (September)
- 2013 Washington State University, Tri-Cities, Richland, Washington, USA; Applied Mathematics seminar (August)
- 2014 New York University, New York, New York, USA; Department of Chemistry seminar (February)
- 2014 Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan; Special seminar (March)
- 2014 Johns Hopkins University, Baltimore, Maryland, USA; Department of Chemistry seminar (October)
- 2014 University of Idaho, Moscow, Idaho, USA; Department of Physics seminar (November)
- 2015 University of Washington, Seattle, WA, USA; Physical Chemistry seminar (April)
- 2015 Brown University, Providence, Rhode Island, USA; Department of Chemistry Colloquium (May)
- 2015 University of Athens, Athens, Greece; Physical Chemistry Seminar (November)
- 2016 Cambridge University, Cambridge, United Kingdom; Department of Chemistry seminar (February)
- 2016 University of Oregon, Eugene, Oregon, USA; Physical Chemistry Colloquium (March)

- 2017 University of Idaho, Moscow, Idaho, USA; Physics Colloquium (April)
- 2017 The Centre for Theoretical and Computational Chemistry, University of Oslo, Oslo, Norway (June). Broadcast at [https://www.youtube.com/watch?v=lq\\_b\\_mT8gWA&feature=youtu.be](https://www.youtube.com/watch?v=lq_b_mT8gWA&feature=youtu.be)
- 2017 Democritus University of Thrace, Alexandroupolis, Greece; Department of Molecular Biology and Genetics, School of Health Sciences Seminar (October)
- 2017 National Centre of Scientific Research "Demokritos", Athens, Greece; Institute of Nanoscience and Nanotechnology (INN) Seminar (October)
- 2017 National Hellenic Research Foundation, Athens, Greece; Theoretical and Physical Chemistry Institute Seminar (October)
- 2018 Stanford University, Menlo Park, California, USA; SLAC National Accelerator Laboratory seminar (February)
- 2018 Lawrence Berkeley National Laboratory, Berkeley, California, USA; seminar (February)
- 2018 Tokyo Institute of Technology, Yokohama, Japan; Institute of Innovative Research, Laboratory for Chemistry and Life Science seminar (March)
- 2018 Ames Laboratory, Ames, Iowa, USA; Division of Chemical and Biological Sciences seminar (September)
- 2019 Tokyo Institute of Technology, Yokohama, Japan; Institute of Innovative Research, Laboratory for Chemistry and Life Science seminar (March)
- 2019 University College London, London, United Kingdom; Thomas Young Centre and Department of Chemistry seminar (April)
- 2019 University of Durham, Durham, UK; Department of Physics Colloquium (June)
- 2019 Tsinghua University, Beijing, China; Department of Chemistry Seminar (August)
- 2020 Tokyo Institute of Technology, Yokohama, Japan; Institute of Innovative Research, World Research Hub Initiative Open Seminar (January)
- 2020 Eidgenössische Technische Hochschule (ETH) Zürich, Switzerland; Laboratory of Physical Chemistry (LPC) Seminar (February)
- 2020 University of Washington, Seattle, WA, USA; Physical Chemistry Colloquium (June)
- 2021 Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA (June)
- 2022 Georgia Institute of Technology (GA Tech) and Emory University, Atlanta, Georgia, USA; Joint Chemistry Colloquium (March)
- 2022 University of Georgia, Athens, Georgia, USA; Chemistry Colloquium (March)
- 2022 Auburn University, Auburn, Alabama, USA; Chemistry Colloquium (March)
- 2022 Fritz Haber Institute of the Max Planck Society, Berlin, Germany; Department of Molecular Physics Seminar (December)
- 2023 East China Normal University, Shanghai, China; School of Chemistry and Molecular Engineering; Honorary Lecture (December)
- 2025 New York University, New York, NY, USA; Simons Center for Computational Physical Chemistry Seminar (January)
- 2025 Institute of Science Tokyo, Tokyo, Japan; World Research Hub Initiative Seminar (November)
- 2025 National and Kapodistrian University of Athens, Athens, Greece; Chemistry Department Seminar (December)

#### Invited Talks in Scientific Conferences/Meetings

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- 1991 *Session chair* in international symposium "*Ab-initio methods in Quantum Chemistry*", Iowa State University, Ames, Iowa, USA (May 9 – 11)
- 1992 *Invited Speaker*, American Chemical Society Northwest Regional Meeting, Missoula, Montana, USA (June 17 – 19)
- 1995 *Invited Speaker*, American Chemical Society National Meeting, Chicago, Illinois, USA (August 20 – 24)

- 1996 *Invited Speaker*, International Symposium of the "Physics and Chemistry of Ice", Hanover, New Hampshire, USA (August 26 – 30)
- 1996 *Invited Plenary Lecture*, Boys-Rahman Medal Award to Enrico Clementi, Royal Society, University College London, United Kingdom (October 3)
- 1996 *Invited Speaker*, Ice Seminar Series, Department of Physics, University of Washington, Seattle, Washington, USA (November)
- 1996 *Session Chair*, "High Pressure and Low Temperature Forms of Ice", International Symposium on the Physics and Chemistry of Ice PCI-96, Hanover, New Hampshire, USA (August 26 – 30)
- 1996 *Member*, Panel Discussion on the "Existence of two kinds of Hydrogen Bond in Ice", International Symposium on the Physics and Chemistry of Ice PCI-96, Hanover, New Hampshire, USA (August 26 – 30)
- 1996 *Invited Speaker*, Fifth Eurasia Conference on Chemical Sciences, Guangzhou, China (December 10 – 14)
- 1997 *Lecturer*, NATO Advanced Study Institute on "Recent Theoretical and Experimental Advances in Hydrogen Bonded Clusters", Elounda, Greece (June 22 – July 4)
- 1998 *Invited Speaker*, Gordon Research Conference on "Molecular Ionic Clusters", Ventura, California, USA (January 4 – 9)
- 1998 *Invited Speaker*, Sanibel Symposium, University of Florida Quantum Theory Project, St. Augustine, Florida, USA (February 21 – 27)
- 1998 *Invited Speaker*, APS National meeting, Los Angeles, California, USA (March 15 – 22)
- 1998 *Invited Speaker*, International symposium "Water in the Gas Phase", Ministry of Research and Education & University of Marne la Vallée, Paris, France (June 21 – 24)
- 1998 *Invited Speaker*, "Large Amplitude Molecular Motion", Telluride Summer Workshop, Telluride Colorado (July 26 – August 1)
- 1999 *Invited Speaker*, "Laser Spectroscopy of Molecular Clusters - Structure and Dynamics", 63<sup>rd</sup> Okazaki Conference, Okazaki, Japan (March 23 – 25)
- 1999 *Invited Speaker*, "International Symposium on Molecular Clusters", Deutsche Forschungsgemeinschaft Schwerpunkt, Niederpöcking by München, Germany (May 25 – 29)
- 1999 *Session Chair*, "International Symposium on Molecular Clusters", Deutsche Forschungsgemeinschaft Schwerpunkt, Niederpöcking by München, Germany (May 25 – 29)
- 1999 *Invited Speaker*, Symposium on "Water and Water Clusters", ACS National meeting, New Orleans, Louisiana, USA (August 26 – 29)
- 1999 *Invited Speaker*, Workshop on "Recent Progress in understanding Water and its implication to the Environmental Research", UMIST, Manchester, United Kingdom (October 20)
- 1999 *Invited Speaker*, International Symposium on "Interplay of Theories and Experiments in Structural Analyses of Molecular Clusters", Institute for Molecular Science, Okazaki, Japan (December 20 – 22)
- 2000 *Chair*, session on "Hydrogen Bonding", Molecular Ionic Clusters (MIC-2000), Toulouse, France (April 16 – 21)
- 2000 *Invited Speaker*, "Water under Extreme Conditions", Telluride Summer Workshop, Telluride Colorado, USA (August 1 – 6)
- 2000 *Invited Speaker*, PacifiChem 2000, Symposium on "Solvated Molecules and Ions: from Clusters to Condensed Phases", Honolulu, Hawaii, USA (December 14 – 19)
- 2001 *Invited Speaker*, American Physical Society (APS) National meeting, Seattle, Washington, USA (March 12 – 16)
- 2001 *Invited Speaker*, 56<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (June 11 – 15)
- 2001 *Session Chair*, Symposium on Water Clusters, 56<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (June 11 – 15)

- 2001 *Invited Speaker*, Computational Chemistry Users Meeting, Molecular Science Computing Facility, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA, USA (June 18 – 19)
- 2001 *Invited Speaker*, American Chemical Society National meeting, Chicago, Illinois, USA (August 26 – 30)
- 2001 *Invited Speaker*, CCP5 meeting, University of Warwick, Warwick, UK (September 16 – 19)
- 2001 *Invited Speaker*, Workshop on Polarizability for Biomolecular Simulation, Snowbird, Utah, USA (December 12 – 14)
- 2002 *Invited Speaker*, Gordon Conference on "*Molecular Ionic Clusters*", Ventura, CA, USA (January 6 – 10)
- 2002 *Invited Speaker*, High Resolution Infrared Spectroscopy Symposium, Pacific Northwest National Laboratory, Richland, WA, USA (April 12 – 13)
- 2002 *Invited Speaker*, Gordon Conference on "*Atomic and Molecular Interactions*", Roger Williams University, Bristol, Rhode Island, USA (July 7 – 12)
- 2002 *Session chair*, American Conference on Theoretical Chemistry (ACTC02), Pittsburgh, Pennsylvania, USA (July 13 – 18)
- 2002 *Invited Speaker*, World Association of Theoretically Oriented Chemists (WATOC02), Lugano, Switzerland (August 4 – 9)
- 2002 *Invited Speaker*, NATO ASI "*Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations*" Rhodes, Greece (September 7 – 15)
- 2003 *Invited Lecture*, EGS (European Geophysical Society) - AGU (American Geological Union) - EUG (European Union of Geosciences) Joint Assembly, Nice, France (April 6 – 11)
- 2003 *Invited Speaker*, Symposium on: "*Mechanics & Physics of Microstructures and Nanostructures - Size Effects*", 5th European Solid Mechanics Conference (EUROMECH), Aristotle University of Thessaloniki, Greece, (August 17 – 22)
- 2003 *Invited Speaker*, Quantum Systems in Chemistry and Physics VIII (QSCP8), Island of Spetses, Greece (August 30 – September 4)
- 2003 *Session Chair*, Quantum Systems in Chemistry and Physics VIII (QSCP8), Island of Spetses, Greece (August 30 – September 4)
- 2004 *Contributed Speaker*, Theory and Applications of Computational Chemistry (TACC2004), Gyeongju Bomum Resort, Korea (February 15 – 20)
- 2004 *Invited Speaker*, American Chemical Society National meeting, Anaheim, California, USA (March 28 – April 1)
- 2004 *Invited Speaker*, Symposium on "*Classical and Quantum Approaches of Rare Event Dynamics in Condensed-Phase Systems*", 87th Canadian Chemistry Conference and Exposition, London, Ontario, Canada (May 29 – June 1)
- 2004 *Invited Speaker*, "*Studies of ice, icy particles, ice surfaces, and ice-adsorbate interactions: a molecular view*", Telluride Summer Workshop, Telluride, Colorado, USA (July 25 – 30).
- 2004 *Invited Speaker*, Gordon Research Conference on "*Water and Aqueous Solutions*", Holderness School, Plymouth, New Hampshire, USA (August 1 – 6)
- 2004 *Discussion Leader*, Session on "*Clusters and Intermolecular Potentials*", Gordon Research Conference on "*Molecular and Ionic Clusters*", Centre Paul Langevin, Aussois, France (September 5 – 10)
- 2004 *Invited Speaker*, 1<sup>st</sup> Condensed Phase and Interfacial Molecular Science (CPIMS) Research Meeting, Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, US Department of Energy, Airlie Conference Center, Warrenton, Virginia, USA (October 24 – 27)
- 2005 *Invited Speaker*, American Chemical Society National meeting, San Diego, California, USA (March 13 – 17)
- 2005 *Invited panel member*, "*Workshop on Interfacial Water*", Sandia National Laboratory, Santa Fe, New Mexico, USA (April 25 – 26)

- 2005 *Invited Speaker*, Environmental Molecular Sciences Institute Annual meeting, Prague, Czech Republic (June 25 – 30)
- 2005 *Session Chair*, Environmental Molecular Sciences Institute Annual meeting, Prague, Czech Republic (June 25 – 30)
- 2005 *Invited Speaker*, “*Dynamics of Molecular Collisions*” DMC 2005, Asilomar, California, USA (July 10 – 15)
- 2005 *Invited Speaker*, Symposium on “*Computational Methods for Atomic and Molecular Clusters*”, International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2005), Loutraki, Greece (October 21 – 26)
- 2005 *Invited Participant*, 9th Annual Chinese – American Frontiers of Science Symposium, US National Academy of Sciences, Xiamen, People’s Republic of China (November 2 – 4)
- 2005 *Invited Speaker*, Pacificchem 2005, Honolulu, HI, USA (December 15 – 20)
- 2006 *Invited Speaker*, Environmental Molecular Sciences Institute Annual meeting, Laguna Beach, CA, USA (January 26 – 27)
- 2006 *Contributed Speaker*, American Physical Society, Baltimore, Maryland, USA (March 13 – 17)
- 2006 *Invited Plenary Lecture*, International Workshop “*Quantitative Quantum Chemistry*”, Santa Fe, New Mexico, USA (March 18 – 20)
- 2006 *Invited Speaker*, American Chemical Society National meeting, Atlanta, Georgia, USA (March 26 – 30)
- 2006 *Invited Speaker*, “*Local Structure and Molecular Scale Properties of Liquid Water*”, Stockholm Discussion Meeting, AlbaNova University Center, Stockholm, Sweden (June 14 – 16)
- 2006 *Invited Speaker*, 11th International Conference of the Physics and Chemistry of Ice, PCI 2006, Bremerhaven, Germany (July 23 – 28)
- 2006 *Session Chair*, Roger E. Miller Memorial Symposium, Univ. of North Carolina at Chapel Hill, Chapel Hill, North Carolina, USA (October 6 – 8)
- 2006 *Invited Keynote Speaker*, New Zealand Institute of Chemistry (NZIC 2006): “*Back to Basics: From Small Molecules to Materials and Surfaces*”, Rotorua, New Zealand (December 2 – 6)
- 2006 *Invited Speaker*, Environmental Molecular Sciences Institute Annual meeting, Christchurch, New Zealand (December 11 – 13)
- 2007 *Invited Speaker*, 4<sup>th</sup> Quantum Life Sciences (QuLiS) symposium on “*Water*”, Hiroshima University, Center of Quantum Life Sciences, Hiroshima, Japan (March 9)
- 2007 *Invited Speaker*, American Chemical Society national meeting, Boston, Massachusetts, USA (August 19 – 23)
- 2007 *Invited Speaker*, 4<sup>th</sup> Condensed Phase and Interfacial Molecular Science (CPIMS) Research Meeting, Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, US Department of Energy, Airlie Conference Center, Warrenton, Virginia, USA (October 22 – 24)
- 2007 *Invited Speaker*, European Science Foundation Conference “*Water Interfaces in Physics, Chemistry and Biology: A multi-disciplinary approach*”, Universitätszentrum Obergurgl, Austria (December 8 – 13)
- 2008 *Invited Speaker*, Environmental Molecular Sciences Institute Annual meeting, Newport Beach, CA, USA (January 23 – 24)
- 2008 *Invited Speaker*, Workshop on “*Aqueous Solutions and Their Interfaces*”, Crete, Greece (June 22 – 27)
- 2008 *Invited Speaker*, Gordon Research Conference on “*Molecular and Ionic Clusters*”, Centre Paul Langevin, Aussois, France (September 7 – 12)
- 2008 *Invited Speaker*, Workshop on “*Water at Biological Interfaces*”, Hangzhou, People’s Republic of China (October 27 – 28)
- 2009 *Invited Speaker*, Environmental Molecular Sciences Institute Annual meeting, Laguna Beach, CA, USA (January 27 – 28)
- 2009 *Plenary Lecture*, Symposium on Size Selected Clusters (S3C) 2009, Brand, Austria (March 8 – 13)

- 2009 *Invited Speaker*, American Chemical Society National meeting, Salt Lake City, Utah, USA (March 22 – 26)
- 2009 *Plenary Lecture*, 31st International Conference on Solution Chemistry, ICSC 2009, Innsbruck, Austria (August 21 – 25)
- 2009 *Session Chair*, 31st International Conference on Solution Chemistry, ICSC 2009, Innsbruck, Austria (August 21 – 25)
- 2009 *Plenary Speaker*, LINKSCEEM (Linking Scientific Computing in Europe and the Eastern Mediterranean), Paphos, Cyprus (October 6 – 8)
- 2010 *Invited Lecture*, AirUCI annual meeting, Laguna Beach, CA, USA (January 20 – 21)
- 2010 *Invited Plenary Lecture*, CECAM workshop on “*Advances in the Implementation of Polarizable Force Fields for Molecular Simulations*”, Lausanne, Switzerland (June 7 – 9)
- 2010 *Session Chair*, CECAM workshop on “*Advances in the Implementation of Polarizable Force Fields for Molecular Simulations*”, Lausanne, Switzerland (June 7 – 9)
- 2010 *Invited Speaker*, “*Many-Body Interactions: From Quantum Mechanics to Force Fields*” Telluride Summer Workshop, Telluride, Colorado, USA (June 14 – 18)
- 2010 *Invited Speaker*, Joint 65th Northwest/22nd Rocky Mountain Regional Meeting (NORM 2010), American Chemical Society, Washington State University, Pullman, Washington, USA (June 20 – 23)
- 2010 *Invited Speaker*, “*Ions in Aqueous Solutions and Molecular Biology: Theory, Simulation, Modeling*” Telluride Summer Workshop, Telluride, Colorado, USA (July 12 – 16)
- 2010 *Invited Speaker*, “*Microscopic Description of Gas Clathrates*”, Telluride Summer Workshop, Telluride, Colorado, USA (July 12 – 16)
- 2010 *Invited Speaker*, American Chemical Society National meeting, Boston, MA, USA (August 22 – 26)
- 2010 *Discussion Leader*, Session on “*Intermolecular Potentials*”, Gordon Research Conference on “*Molecular and Ionic Clusters*” (MIC 2010), Atama Kougen Resort Hotel Belnatio, Niigata, Japan (September 5 – 10)
- 2010 *Plenary Lecture*, 11<sup>th</sup> Eurasia Conference of Chemical Sciences, Dead Sea, Jordan (October 6 – 10)
- 2010 *Invited Speaker*, Nanothailand 2010, Thailand Science Park Convention Center (NSTDA), Pathumthani, Thailand (November 18 – 20)
- 2010 *Invited Speaker*, Technical Symposium “*Anharmonic Vibrations of Molecules and Clusters: Experiment and Theory*”, PacifiChem 2010, Honolulu, HI, USA (December 15 – 20)
- 2011 *Invited Speaker*, Collaborative Workshop in Chemistry at the Interfaces, University of California Irvine, Laguna Beach, California, USA (January 19 – 20)
- 2011 *Invited Speaker*, 7<sup>th</sup> Condensed Phase and Interfacial Molecular Science (CPIMS) Research meeting, Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, US Department of Energy, Hyatt Regency, Baltimore, MD (June 12 – 15)
- 2011 *Invited Lecture*, Ninth triennial congress of the World Association of Theoretical and Computational Chemists (WATOC), Santiago de Compostela, Spain (July 17 – 22)
- 2011 *Invited Speaker*, 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Waseda University, Tokyo, Japan (September 2 – 8)
- 2011 *Session Chair*, 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Waseda University, Tokyo, Japan (September 2 – 8)
- 2012 *Invited Speaker*, Collaborative Workshop in Chemistry at the Interfaces, University of California Irvine, Laguna Beach, California, USA (January 26 – 27)
- 2012 *Invited Speaker*, Gordon Research Conference on “*Molecular and Ionic Clusters*”, Ventura, CA USA (January 29 – February 3)
- 2012 *Invited Speaker*, American Chemical Society National meeting, San Diego, CA, USA (March 25 – 29)
- 2012 *Invited Speaker*, 12th Eurasia Conference on Chemical Sciences, Corfu, Greece (April 16 – 21)
- 2012 *Session Chair*, 12th Eurasia Conference on Chemical Sciences, Corfu, Greece (April 16 – 21)

- 2012 *Invited Speaker*, Gordon Research Conference on “*Computational Chemistry*”, Mount Snow, VT USA (July 22 – 27)
- 2012 *Invited Speaker*, American Chemical Society National meeting, Philadelphia, PA, USA (August 19 – 23)
- 2013 *Invited Speaker*, Collaborative Workshop in Chemistry at the Interfaces, University of California Irvine, Laguna Beach, California, USA (January 31 – February 1)
- 2013 *Invited Speaker*, Gordon Conference on “*Gaseous Ions: Structures, Energetics and Reactions*”, Galveston, TX, USA (February 24 – March 1)
- 2013 *Invited Speaker*, American Chemical Society National meeting, New Orleans, LA, USA (April 7 – 11)
- 2013 *Invited Speaker*, “*Water at Interfaces: New Developments in Physics, Chemistry and Biology*”, Ecole de Physique, Les Houches, France (April 15 – 26)
- 2013 *Invited Speaker* International Conference on Theoretical and High-Performance Computational Chemistry 2013 (ICT-HPCC13), Dalian, China (July 21 – 25)
- 2013 *Session Chair*, American Chemical Society National meeting, Indianapolis, IN, USA (September 8 – 12)
- 2013 *Invited Speaker*, in “*Large Scale Production Computing and Storage Requirements for Basic Energy Sciences: Target 2017*”, DOE Program Review, Washington DC, USA (October 8 – 9)
- 2013 *Invited Speaker*, 9<sup>th</sup> Condensed Phase and Interfacial Molecular Science (CPIMS) Research meeting, Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, US Department of Energy, Bolger Conference Center, Potomac, MD, USA (October 21 – 23)
- 2014 *Invited Speaker*, Collaborative Workshop in Chemistry at the Interfaces, University of California Irvine, Laguna Beach, California, USA (January 22 – 23)
- 2014 *Invited Speaker*, Symposium on “*Molecular Science and Synthesis of Functional Molecules for Next Generation*”, Hiroshima University, Hiroshima, Japan (March 10 – 11)
- 2014 *Invited Speaker*, American Chemical Society National meeting, Dallas, TX, USA (March 16 – 20)
- 2014 *Discussion Leader*, session on “*Theoretical Approaches to Interactions in Clusters*”, Gordon Research Conference on “*Molecular and Ionic Clusters*”, Il Ciocco Resort, Lucca (Barga), Italy (April 27 – May 2)
- 2014 *Invited Speaker*, 3<sup>rd</sup> Changsha International Workshop on Theoretical and Computational Chemistry with Materials (TCC-III), Changsha, Hunan, China (June 8 – 10)
- 2014 *Invited Lecture*, American Conference of Theoretical Chemistry (ACTC 2014), Telluride, Colorado, USA (July 21 – 24)
- 2014 *Invited Speaker*, International Conference on Chemical Bonding (ICCB 2014), Kauai, Hawaii, USA (July 24 – 28)
- 2014 *Invited Speaker*, American Chemical Society National meeting, San Francisco, CA, USA (August 10 – 14)
- 2014 *Session Chair*, American Chemical Society National meeting, San Francisco, CA, USA (August 10 – 14)
- 2014 *Invited Speaker*, NORDITA Conference on Water, Stockholm, Sweden (October 13 – 21)
- 2014 *Invited Speaker*, 10<sup>th</sup> Condensed Phase and Interfacial Molecular Science (CPIMS) Research meeting, Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, US Department of Energy, Bolger Conference Center, Potomac, MD, USA (October 20 – 22)
- 2015 *Invited Speaker*, Workshop on Fundamental Challenges in our Understanding of the Physics and Chemistry of Water, University of Houston, Houston, Texas, USA (January 16 – 17)
- 2015 *Invited participant*, National Science Foundation (NSF) workshop on the Conceptualization of a new Software Institute, Houston, Texas, USA (January 22 – 24)
- 2015 *Invited Speaker*, American Physical Society national meeting, San Antonio, Texas, USA (March 2 – 6)

- 2015 *Invited Tutorial*, National Science Foundation (NSF) workshop on “*Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions*”, Washington DC, USA (May 31 – June 4)
- 2015 *Invited Speaker*, symposium on “*Clathrate Hydrates Fundamentals: Bridging Molecular Structures to Microscopic Properties and Behavior*”, Telluride Summer Workshop, Telluride, Colorado, USA (July 6 – 10)
- 2015 *Invited Speaker*, symposium entitled “*Developments of spectroscopic investigation of intermolecular interactions and dynamics of molecular clusters*”, International Chemical Congress of Pacific Basin Societies (Pacifichem 2015), Honolulu, Hawaii, USA (December 15 – 20)
- 2015 *Invited Speaker*, symposium entitled “*Chemistry of Atmospheric Aerosols*”, International Chemical Congress of Pacific Basin Societies (Pacifichem 2015), Honolulu, Hawaii, USA (December 15 – 20)
- 2015 *Invited Speaker*, symposium entitled “*Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities*”, International Chemical Congress of Pacific Basin Societies (Pacifichem 2015), Honolulu, Hawaii, USA (December 15 – 20)
- 2016 *Invited Panelist*, Gordon Research Seminar (GRS) on “*Molecular and Ionic Clusters*”, Ventura, California, USA (January 16 – 17)
- 2016 *Invited Speaker*, Gordon Research Conference on “*Molecular and Ionic Clusters*”, Ventura, California, USA (January 17 – 22)
- 2016 *Invited Speaker*, American Chemical Society National meeting, San Diego, CA, USA (March 13 – 17)
- 2016 *Session Chair*, American Chemical Society National meeting, San Diego, CA, USA (March 13 – 17)
- 2016 *Session Chair*, CECAM Workshop “*Computational methods for modeling multiply-charged droplets*”, CECAM-HQ-EPFL, Lausanne, Switzerland (July 6 – 8)
- 2016 *Invited Speaker*, Gordon Research Conference on “*Molecular Interactions and Dynamics*”, Stonehill College, Easton, Massachusetts, USA (July 10 – 15)
- 2016 *Invited Speaker*, Gordon Research Conference on “*Water and Aqueous Solutions*”, Holderness School, Holderness, New Hampshire, USA (July 31 – August 5)
- 2016 *Invited Speaker*, American Chemical Society National meeting, Philadelphia, PA, USA (August 21 – 26)
- 2016 *Session Chair*, “*Future of Chemical Physics*”, The Journal of Chemical Physics, University of Oxford, UK (August 31 – September 2)
- 2016 *Session Chair*, “*Recent Progresses on the Experimental & Theoretical-Computational Techniques for the Study of Liquids and Supercritical Fluids: From Simple to Complex*”, European Molecular Liquids Group/Japanese Molecular Liquids Group (EMLG/JMLG) annual meeting, Platania, Crete, Greece (September 11 – 16)
- 2016 *Invited Speaker*, Symposium on “*Energy and Sustainable Materials*”, University of Oregon, Eugene, Oregon, USA (September 30 – October 2)
- 2016 *Invited Speaker*, 12<sup>th</sup> Condensed Phase and Interfacial Molecular Science (CPIMS) Research meeting, Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, US Department of Energy, Gaithersburg, MD, USA (November 1 – 4)
- 2017 *Invited Speaker*, “*GAMESS7557SSEMAG Palindromic Theory Symposium*”, Aqua Kauai Beach Resort, Lihue, Kauai, USA (January 16 – 18)
- 2017 *Invited Speaker*, “*Roma Tre Congress of Water under Extreme Conditions*”, Rome, Italy (June 14 – 16)
- 2017 *Session chair*, “*Roma Tre Congress of Water under Extreme Conditions*”, Rome, Italy (June 14 – 16)
- 2017 *Invited Speaker*, 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2017), Munich, Germany (August 27 – September 1)
- 2017 *Session Chair*, 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2017), Munich, Germany (August 27 – September 1)
- 2018 *Invited Speaker*, XXI Symposium on Atomic, Cluster and Surface Physics (SASP), University of Innsbruck, Universitätszentrum Obergurgl, Austria (February 11 – 16)

- 2019 *Plenary Lecture*, 59<sup>th</sup> Sanibel Symposium (February 17 – 22)
- 2019 *Discussion Leader*, session “*In Silico Investigations*”, Gordon Research Conference “Gaseous Ions: Structures, Energetics, and Reactions”, Ventura, CA, USA (February 17 – 22)
- 2019 *Invited Speaker*, workshop on “*Intermolecular Interactions: New Challenges for Ab Initio Theory*”, Telluride Science Research Center, Telluride, Colorado, USA (March 18 – 2)
- 2019 *Headline Invited Speaker*, Faraday Discussion of the Royal Society: “*Advances in Ion Spectroscopy: From Astrophysics to Biology*”, York, United Kingdom (April 8 – 10)
- 2019 *Invited Speaker*, 102<sup>nd</sup> Canadian Chemistry Conference and Exhibition, Québec City, Quebec, Canada (June 3 – 7)
- 2019 *Invited Speaker*, “Roma Tre Congress of Water under Extreme Conditions”, Rome, Italy (June 12 – 14)
- 2019 *Invited Speaker*, International Symposium “*Highly-excited States, Many-body and Non-covalent Interactions*”, University of Manchester, Manchester, United Kingdom (June 19 – 21)
- 2019 *Keynote Lecture*, International Symposium of Theoretical and Physical Chemistry (ISTPC-2019), Southern University of Science and Technology (SUSTech), Shenzhen, China (July 28 – 30)
- 2019 *Invited Speaker*, American Chemical Society National meeting, San Diego, CA, USA (August 25 – 29)
- 2019 *Keynote Speaker*, “*Renewable-Gas Workshop: Prospects, Challenges and Outlook*”, University College Dublin, Dublin, Ireland (September 13)
- 2020 *Discussion Leader*, Gordon Research Conference “Molecular and Ionic Clusters”, Ventura, CA, USA (January 26 – 31)
- 2020 *Session Chair*, XXII Symposium on Atomic, Cluster and Surface Physics (SASP2020), St. Moritz, Switzerland (February 2 – 7)
- 2021 *Session Chair*, Technical Symposium “*Structure and Function of Complex Molecular Clusters – Challenges in Theory and Experiment*”, PacificChem 2020, Honolulu, Hawaii, USA (December 15 – 20)
- 2021 *Invited Talk*, Technical Symposium “*Structure and Function of Complex Molecular Clusters – Challenges in Theory and Experiment*”, PacificChem 2020, Honolulu, Hawaii, USA (December 15 – 20)
- 2022 *Invited Plenary Lecturer*, “*Modern Topics in Chemical Physics*”, Department of Dynamics at Surfaces Workshop, University of Gottingen and Max Planck Institute for Multidisciplinary Sciences, Franken Akademie Schloß Schney, Lichtenfels, Germany (May 11 – 14)
- 2022 *Invited Speaker*, 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, BC, Canada (July 3 – 8)
- 2022 *Invited Speaker*, Gordon Research Conference on “*Computational Chemistry: Multiscale Modeling of Complex Systems: Methods and Applications*”, Castelldefels, Spain (July 17 – 22)
- 2022 *Keynote Lecture*, 3rd International Symposium of JSPS Core-to-Core Program on “*Molecular Recognition Mechanism between Flexible Molecules*”, Tokyo Institute of Technology, Tokyo, Japan (September 29)
- 2023 *Invited Speaker*, European Conference on Computational and Theoretical Chemistry (EuChemS CompChem 2023) “*Exploring Molecular Space*”, Thessaloniki, Greece (August 27 – 31)
- 2023 *Invited Speaker*, The Inaugural Lennard-Jones Centre meeting, “*Theory and Molecular Simulation in the Physical Sciences*”, University of Cambridge, Cambridge, UK (September 4 – 8)
- 2023 *Invited Speaker*, the 5<sup>th</sup> International Symposium of Japan Society for the Promotion of Science (JSPS) Core-to-Core Program on “*Molecular Recognition Mechanism between Flexible Molecules*”, Technical University of Berlin, Germany (October 16 – 20)
- 2023 *Invited Speaker*, the 9<sup>th</sup> Asian Conference on Colloid and Interface (ACCIS 2023), Chinese University of Hong Kong, Hong Kong, SAR (December 12 – 15)
- 2024 *Invited Speaker*, American Chemical Society National meeting, New Orleans, LA, USA (March 17 – 21)

- 2024 *Invited Speaker*, XXI<sup>st</sup> International Workshop on Quantum Atomic and Molecular Tunneling Systems (QAMTS24), Palacio Miramar, Donostia - San Sebastián, Spain (June 16 – 21)
- 2024 *Invited Speaker*, 78<sup>th</sup> Northwest Regional Meeting (NORM), Washington – Idaho Border Section of the American Chemical Society, Washington State University, Pullman, WA, USA (June 23 – 26)
- 2024 *Invited Speaker*, Gordon Research Conference on “*Molecular Interactions and Dynamics*”, Stonehill College, Easton, Massachusetts, USA (July 7 – 12)
- 2024 *Invited Speaker*, 7th International Symposium of JSPS Core-to-Core Program on “*Molecular Recognition Mechanism between Flexible Molecules*” Tokyo Institute of Technology, Tokyo, Japan (July 29 – August 2)
- 2024 *Invited Speaker*, “*ERC n-AQUA Workshop*”, Kalamata, Greece (September 23 – 28)
- 2025 *Invited Speaker*, “*From ab initio Computations to Conceptual Insights into Bonding*”, Telluride Workshop, Telluride, Colorado, USA (May 27 – 31)
- 2025 *Invited Speaker*, “*Aqueous Systems: The Frontier and Beyond*”, Kalamata, Greece (June 15 – 21)
- 2025 *Invited Speaker*, Core-to-core Symposium UCSD – SPS, “*Elucidation of solvation effects on molecular recognition*”, Santa Barbara, California, USA (September 15 – 17)
- 2025 *Invited Speaker*, “*Synergy of Theory and Experiments in Exploring Molecular Functionality in Supramolecules and Molecular Clusters in the Gas Phase*”, Pacificchem 2020, Honolulu, Hawaii, USA (December 15 – 20)
- 2025 *Session Chair*, “*Synergy of Theory and Experiments in Exploring Molecular Functionality in Supramolecules and Molecular Clusters in the Gas Phase*”, Pacificchem 2020, Honolulu, Hawaii, USA (December 15 – 20)
- 2026 *Invited Speaker*, Gordon Research Conference on “*Molecular and Ionic Clusters*”, Renaissance Tuscany Il Ciocco, Lucca (Barga), Italy (April 19 – 24)
- 2026 *Invited Speaker*, “*Water@Nature, 6<sup>th</sup> edition of the International Workshop WaterX: Exotic Properties of Water Under Extreme Conditions*”, Circolo Ufficiali della Marina, La Maddalena Island, Sardinia, Italy (May 24 – 29)
- 2026 *Invited Speaker*, “*Water anomalies - origin and implications*”, Stockholm, Sweden (June 8 – 12)
- 2026 *Invited Speaker*, “*International Conference of Molecular Electronic Structure 2026 (MES2026)*”, Kamena Vourla, Greece (September 19 – 23)

### Contributed talks in Scientific Conferences/Meetings

- 1986 *Poster presentation*, 19<sup>th</sup> Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, USA (May 15 – 17)
- 1987 *Two poster presentations*, American Conference on Theoretical Chemistry, Gull Lake, Minnesota, USA (July 27 – 31)
- 1988 *Poster presentation*, 21<sup>st</sup> Midwest Theoretical Chemistry Conference, Argonne National Laboratory, Argonne, Illinois, USA (May 12 – 14)
- 1988 *Attended*, “*Computational Chemistry on Supercomputers: Algorithms and Methods*”, Center for High Performance Computing, University of Texas, Austin, Texas, USA (October 5– 8)
- 1989 *Attended*, “*Parallel Computers in Chemistry*”, Argonne National Laboratory, Argonne, Illinois, USA (June 12 – 16)
- 1990 *Oral presentation*, West Coast Theoretical Chemistry Conference, University of Utah, Salt Lake, Utah, USA (March 23 – 25)
- 1990 *Poster presentation*, ACS Spring meeting, Boston, Massachusetts, USA (April 22 – 27)
- 1991 *Poster presentation*, West Coast Theoretical Chemistry Conference, NASA Ames Research Center, Moffett Field, California, USA (March 27 – 29)
- 1991 *Oral presentation*, West Coast Theoretical Chemistry Conference, NASA Ames Research Center, Moffett Field, California, USA (March 27 – 29)
- 1991 *Poster presentation and poster contribution* in international symposium “*Ab-initio methods in Quantum Chemistry*”, Iowa State University, Ames, Iowa, USA (May 9 – 11)

- 1991 *Invited Talk Contribution*, Energy Research Power Supercomputer Users Symposium, Gaithersburg, Maryland, USA (May 20 – 22)
- 1992 *Poster presentation*, Second Symposium on Molecular Reactions Dynamics in Condensed Matter, Irvine, California, USA (April 2 – 4)
- 1992 *Poster presentation*, American Chemical Society national meeting, San Francisco, California, USA (April 5 – 10)
- 1992 *Poster presentation*, 13<sup>th</sup> West Coast Theoretical Chemistry Conference, Pacific Northwest Laboratory, Richland, Washington, USA (May 21 – 23)
- 1992 *Poster presentation*, NATO ASI on "Molecular Spectroscopy: Recent Experimental and Computational Advances", Ponta Delgada, Açores, Portugal (August 29 – September 11)
- 1993 *Oral presentation*, 14<sup>th</sup> West Coast Theoretical Chemistry Conference, Univ. of California, Los Angeles, California, USA (June 17 – 19)
- 1993 *Poster presentation*, American Conference on Theoretical Chemistry, Rochester, New York, USA (June 28 – July 2)
- 1993 *Oral presentation*, American Chemical Society National Meeting, Chicago, Illinois, USA (August 22 – 28)
- 1994 *Three poster presentations*, American Chemical Society National Meeting, San Diego, California, USA (March 13 – 18)
- 1994 *Poster presentation*, 8<sup>th</sup> International Congress of Quantum Chemistry, Prague, Czech Republic (June 19 – 23)
- 1994 *Contribution*, CCP5 meeting on "How to Derive the Interatomic Potentials Needed for Simulation Studies", Mansfield College, Oxford, United Kingdom (July 4 – 5)
- 1995 *Poster presentation*, American Physical Society, San Jose, California, USA (March 20 – 25)
- 1995 *Poster presentation*, 16<sup>th</sup> West Coast Theoretical Chemistry Conference, San Diego Supercomputer Center, California, USA (March 29 – 31)
- 1995 *Poster presentation*, American Chemical Society National Meeting, Anaheim, California, USA (April 2 – 6)
- 1995 *Attended*, NATO Advanced Study Institute (ASI) on "Photonic Band Gap Materials", Elounda, Greece (June 19 – 30)
- 1996 *Poster presentation*, West Coast Theoretical Chemistry Conference, University of Nevada-Las Vegas, Las Vegas, Nevada, USA (April 3 – 5)
- 1996 *Poster presentation*, Gordon Research Conference on "Molecular Ionic Clusters", Il Ciocco, Lucca (Barga), Italy (May 5 – 10)
- 1999 *Poster presentation*, Gordon Research Conference on "Structures, Energetics and Dynamics of Gaseous Ions", Ventura, California, USA (February 28 – March 4)
- 1999 *Contributed Oral Presentation*, APS National Meeting, Atlanta, Georgia, USA (March 20 – 26)
- 2000 *Poster Contribution*, Fifth Workshop "Quantum Systems in Chemistry and Physics", Uppsala, Sweden (April 13 – 18)
- 2000 *Invited Talk Contribution*, 55<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (June)
- 2001 *Presentation*, 56<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (June 11 – 15)
- 2002 *Contributed Talk*, National Laboratory Catalysis Conference (NLCat 2002), Pacific Northwest National Laboratory, Richland, Washington USA (May 22 – 23)
- 2002 *Contributed Talk*, 57<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (June 17 – 21)
- 2002 *Contributed Talk*, Division of Fuel Chemistry, 224<sup>th</sup> ACS National Meeting, Boston, Massachusetts, USA (August 18 – 22)
- 2005 *Poster presentation*, Symposium on Size Selected Clusters (S3C), Brand, Austria (February 28 – March 3)

- 2007 *Contributed Talk*, American Chemical Society Midwest Regional meeting, Kansas City, Missouri (November 7 – 10)
- 2009 *3 Poster presentations*, Symposium on Size Selected Clusters (S3C) 2009, Brand, Austria (March 8 – 13)
- 2009 *Contributed Talk*, American Chemical Society National meeting, Salt Lake City, Utah, USA (March 22 – 26)
- 2009 *3 Poster presentations*, American Chemical Society National meeting, Salt Lake City, Utah, USA (March 22 – 26)
- 2009 *Contributed talk*, XVIII International Conference on "Horizons in Hydrogen Bond Research", Paris, France (September 14 – 18)
- 2010 *Contributed Poster*, Faraday Discussion FD146 "Wetting Dynamics of Hydrophobic and Structured Surfaces", Richmond, Virginia, USA (April 12 – 14)
- 2010 *Contributed Talk*, 65th International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (June 16 – 20)
- 2010 *Contributed Oral presentation*, 17th International Conference on Ultrafast Phenomena, Snowmass, CO, USA (July 18 – 23)
- 2011 *Contributed Plenary Lecture*, 66th Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (June)
- 2013 *Contributed Oral Presentation*, 2nd European Optical Society Conference on Optofluidics (EOSOF 2013), Munich, Germany (May 13 – 15)
- 2013 *Contributed Oral Presentation*, "Intermolecular Interactions: New Challenges for Ab Initio Theory", Telluride Summer Workshop, Telluride, Colorado, USA (July 15 – 19)
- 2013 *Contributed Talk*, International Society for Optics and Photonics (SPIE), San Diego, California (August 25 – 29)
- 2013 *Contributed Talk*, American Chemical Society National meeting, Indianapolis, Indiana, USA (September 8 – 12)
- 2013 *Contributed Talk*, Materials Research Society (MRS) Fall Meeting and Exhibit, Boston, Massachusetts, USA (December 1 – 6)
- 2014 *Contributed Talk*, Collaborative Workshop in Chemistry at the Interfaces, University of California Irvine, Laguna Beach, California, USA (January 22 – 23)
- 2014 *Contributed Talk*, Conference on Lasers and Electro-Optics (CLEO) 2014, San Jose, California, USA (June 8 – 13)
- 2014 *Contributed Poster*, Midwest Theoretical Chemistry Conference, Northwestern University, Chicago, Illinois, USA (June 15 – 17)
- 2014 *Contributed Poster*, American Conference of Theoretical Chemistry (ACTC 2014), Telluride, Colorado, USA (July 21 – 24)
- 2014 *Contributed Talk*, Materials Research Society (MRS) Fall Meeting & Exhibit, Boston, Massachusetts, USA (November 30 – December 5)
- 2015 *Two contributed Talks*, 70<sup>th</sup> International Symposium on Molecular Spectroscopy, Urbana – Champaign, Illinois, USA (June 22 – 26)
- 2016 *Contributed Talk*, 71<sup>st</sup> International Symposium on Molecular Spectroscopy, Urbana – Champaign, Illinois, USA (June 20 – 24)
- 2017 *Poster Presentation*, Gordon Conference on "Gaseous Ions: Structures, Energetics & Reactions", Ventura Beach Marriott, Ventura, California, USA (February 12 – 17)
- 2017 *Contributed Talk*, 4th Conference on Optofluidics, Munich, Germany (June)
- 2017 *Contributed Poster Presentation*, 1st Northwest Theoretical Chemistry Conference (NWTCC), Pacific Northwest National Laboratory, Richland, WA, USA (October)
- 2018 *Contributed Poster Presentation*, Gordon Conference on "Molecular and Ionic Clusters", Renaissance Tuscany Il Ciocco, Lucca (Barga), Italy (February)
- 2019 *Poster Presentation*, Exascale Computing Project Annual meeting, Houston, Texas, USA (January 14 – 18)

- 2019 *Oral Presentation*, 2<sup>nd</sup> Northwest Theoretical Chemistry Conference (NWTCC), Washington State University, Pullman, WA, USA (June 14 – 15)
- 2019 *Contributed presentation*, Symposium on “*Interface between experiments and modeling in unraveling the physical and chemical properties of charged droplets*”, American Chemical Society National meeting, San Diego, CA, USA (August 25 – 29)
- 2020 *Contributed presentation*, CoDA 2020, Santa Fe, NM, USA (February 26)
- 2020 *Contributed presentation*, Machine Learning and the Physical Sciences - Workshop at the 34th Conference on Neural Information Processing Systems (NeurIPS) (December 11)
- 2020 *Contributed presentation*, 3rd RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry, Online Conference, United Kingdom (September 28)
- 2022 *Contributed presentation*, Symposium on “*Drug Design: Molecular Dynamics and their Mechanism*”, American Chemical Society National meeting, San Diego, CA, USA (March 20 – 24)
- 2022 *2 Contributed presentations*, Symposium on “*New Developments in Hybrid QM/QM, QM/MM, and Fragmentation Methods*”, American Chemical Society National meeting, San Diego, CA, USA (March 20 – 24)
- 2022 *Contributed presentation*, International Symposium on Molecular Spectroscopy, University of Illinois at Urbana Champaign, IL, USA (June 20 – 24)
- 2022 *3 Contributed poster presentations*, 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, BC, Canada (July 3 – 8)

### Organization of Scientific Conferences/Meetings

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- 1995 *Organizer*, Workshop “*Nature of Hydrogen Bonding in Ice and Water*”, Pacific Northwest National Laboratory, Richland, Washington, USA (September 25)
- 1997 *Director*, NATO Advanced Study Institute (ASI) on “*Recent Theoretical and Experimental Advances in Hydrogen Bonded Clusters*”, Elounda, Crete, Greece (June 22 – July 4)
- 1998 *Organizer*, Workshop “*Ice Physics and Chemistry: Environmental Impacts*”, Pacific Northwest National Laboratory, Richland, Washington, USA (August 13 – 14)
- 2003 *Organizing Committee*, “*Quantum Systems in Chemistry and Physics VIII*”, Spetses Island, Greece (August 30 - September 4)
- 2004 *Vice-chair*, Gordon Research Conference “*Molecular and Ionic Clusters*”, Centre Paul Langevin, Aussois, France (September 5 – 10)
- 2006 *Co-Chair* (with M. A. Duncan, Univ. of Georgia, USA), Gordon Research Conference “*Molecular and Ionic Clusters*”, Ventura, California, USA (February 19 – 24)
- 2008 *Co-organizer* (with G. A. Voth, Univ. of Utah, USA), International Workshop on “*Aqueous Solutions and Their Interfaces*”, Crete, Greece (June 22 – 27)
- 2010 *Co-organizer* (with H. Kjaergaard, S.-I. Ishiuchi, D. McNaughton), Technical Symposium “*Anharmonic Vibrations of Molecules and Clusters: Experiment and Theory*”, PacifiChem 2010, Honolulu, Hawaii, USA (December 15 – 20)
- 2013 *Co-organizer* (with R. J. Saykally, Univ. of California Berkeley, USA), Symposium on “*Theory and Experiment on Water and hydration*”, American Chemical Society National meeting, Indianapolis, Indiana, USA (September 8 – 12)
- 2016 *Co-organizer* (with S. Consta, M. A. Miller and M.-P. Gaigeot) CECAM Workshop “*Advances in computational methods for modeling multiply charged drops*”, Lausanne, Switzerland (July 5 – 8)
- 2016 *International Advisory Committee*, International Conference on “*Theory and Applications of Computational Chemistry (TACC) 2016*”, University of Washington, Seattle, Washington, USA (August 30 – September 4)
- 2016 *Co-organizer* (with J. Samios, Univ. of Athens, Greece, and W. Schroer, Bremen Univ., Germany), “*Recent Progresses on the Experimental & Theoretical-Computational Techniques for the Study of Liquids and Supercritical Fluids: From Simple to Complex*”, European Molecular Liquids

- Group/Japanese Molecular Liquids Group (EMLG/JMLG) annual meeting, Platanias, Crete, Greece (September 11 – 16)
- 2017 *Co-organizer* (with G. K. Schenter, PNNL), “1st Northwest Theoretical Chemistry Conference (NWTCC)”, Pacific Northwest National Laboratory, Richland, WA, USA (October 26 – 28)
- 2018 Chair, Physical and Computational Chemistry track, ACS Northwest Regional Meeting (NORM 2018), Richland, WA, USA (June 24 – 27)
- 2018 *Co-organizer* (with D. J. Wales, Cambridge University, UK), “Energy Landscapes 2018”, Kalamata, Greece (September 2 – 9)
- 2019 *Co-organizer* (with S. Consta, Western Ontario University, Canada), Symposium on “Interface between experiments and modeling in unraveling the physical and chemical properties of charged droplets”, American Chemical Society National meeting, San Diego, CA, USA (August 25 – 29)
- 2019 *Co-organizer* (with N. Govind, PNNL; J. R. Rehr, University of Washington; K. Gaffney, SLAC; F. Villa, University of Washington), Workshop on “Developments & Challenges in X-ray Spectroscopies and Ultrafast Dynamics: Experiment and Theory”, 2019 SSRL/LCLS Users’ Meeting, SLAC National Accelerator Laboratory, Stanford University, Menlo Park, CA, USA (September 24 – 27)
- 2021 *Co-organizer* (with S. Consta), Technical Symposium “Chemistry in Small Volumes”, International Union of Pure and Applied Chemistry (IUPAC) / Canadian Chemistry Conference and Exhibition (CCCE), Montreal, CA, USA (August 13 – 20)
- 2021 *Co-organizer* (with M. Fujii, A. Fujii, E. Bieske, L. Jiang), Technical Symposium “Structure and Function of Complex Molecular Clusters – Challenges in Theory and Experiment”, PacificChem 2020, Honolulu, Hawaii, USA (December 15 – 20)
- 2023 *Co-organizer* (with S. Choudhury), Workshop “AI in the Physical Sciences”, Pacific Northwest National Laboratory, Richland, WA, USA (March 13 – 14)
- 2024 *Co-organizer* (with Mischa Bonn, Lydéric Bocquet, Angelos Michaelides), “ERC n-AQUA Workshop”, Kalamata, Greece (September 23 – 28)
- 2025 *Co-organizer* (with G. A. Voth), International Conference “Aqueous Systems: The Frontier and Beyond”, Kalamata, Greece (June 16 – 21)
- 2025 *Co-organizer* (with M. S. de Vries, S.-I Ishiuchi, O. Dopfer, A. Zehnacker-Rentien), Core-to-core Symposium UCSD – SPS, “Elucidation of solvation effects on molecular recognition”, Santa Barbara, California, USA (September 15 – 17)
- 2025 *Co-organizer* (with A. Fujii, E. Bieske, S.-I Ishiuchi, L. Jiang, Y. Ohshima, Y. Xu), Technical Symposium “Synergy of Theory and Experiments in Exploring Molecular Functionality in Supramolecules and Molecular Clusters in the Gas Phase”, Pacificchem 2025, Honolulu, Hawaii, USA (December 15 – 20)

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## PUBLICATIONS OF SOTIRIS S. XANTHEAS

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### A. Book Editor

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1. "Recent Experimental and Theoretical Advances in Hydrogen Bonded Clusters", NATO ASI Series C, Mathematical and Physical Sciences 561, S. S. Xantheas (Ed.), Kluwer Academic Publishers, Dordrecht, The Netherlands (2000)

### B. Chapters in Books

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2. **S. S. Xantheas** and T. H. Dunning, Jr., "Ab-initio Characterization of Water and Negative Ion-Water Clusters" in *Advances in Molecular Vibrations and Collision Dynamics*, Z. Bacic and J. M. Bowman (editors), vol. 3, JAI press, pp. 281-309 (1998)
3. **S. S. Xantheas**, "Cooperative Effects in Water Clusters", in *Recent Experimental and Theoretical Advances in Hydrogen Bonded Clusters*, NATO ASI Series C, Mathematical and Physical Sciences 561, S. S. Xantheas (Ed.), pp. 119-128, Kluwer Academic Publishers, Dordrecht, The Netherlands (2000)
4. **S. S. Xantheas**, "Intermolecular Interactions and Cooperative Effects from Electronic Structure Calculations: An Effective Means for Developing Interaction Potentials for Condensed Phase Simulations" in *Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations*, NATO Science Series II: Mathematics, Physics and Chemistry vol. 133 J. Samios and V. A. Durov (Eds.), pp. 1-15, Kluwer Academic Publishers, Dordrecht, The Netherlands (2004)
5. **S. S. Xantheas**, "Interaction potentials for water from accurate cluster calculations" in *Structure and Bonding: Intermolecular Forces and Clusters II*, Springer-Verlag Berlin Heidelberg, D. J. Wales (Editor), vol. **116**, pp. 119 – 148 (2005)
6. S. Yoo and **S. S. Xantheas**, "Structures, Energetics and Spectroscopic Fingerprints of Water Clusters  $n=2-24$ " in *Handbook of Computational Chemistry*, J. Leszczynski (ed.), Springer Science+Business Media B. V., ISBN 978-94-007-0710-8, Chapter 21, pp. 761 – 792 (2012)
7. S. Yoo and **S. S. Xantheas**, "Structures, Energetics and Spectroscopic Fingerprints of Water Clusters  $n=2-24$ " in *Handbook of Computational Chemistry*, J. Leszczynski (editor), 2nd Edition, Springer International Publishing Switzerland, ISBN 978-3-319-27281-8, Chapter 26, pp. 1139 – 1175 (2017)

### C. Conference Proceedings

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8. T. H. Dunning, Jr., **S. S. Xantheas**, A. C. Hess, D. F. Feller, R. A. Kendall and R. L. Ornstein, "Modeling Molecular Processes in the Environment", in *Proceedings of the First Energy Research Power Supercomputer Users Symposium*, U. S. Department of Energy, Gaithersburg, Maryland, USA, May 21 – 22 (1991)
9. E. Aprà, R. J. Harrison, W. A. deJong, A. P. Rendell, V. Tipparaju, **S. S. Xantheas**, "Liquid Water: Obtaining the right answer for the right reasons", *SC'09: Proceedings of the Conference on High Performance Computing, Networking, Storage and Analysis*, SESSION: Gordon Bell finalists, article No. 66, Published by ACM, New York, NY USA (2009). ISBN:978-1-60558-744-8. DOI: <http://doi.acm.org/10.1145/1654059.1654127>
10. J. C. Werhahn, S. Pandelov, S. Yoo, **S. S. Xantheas**, H. Iglev, "Dynamics of Confined Water Molecules in Aqueous Salt Hydrates", in *Ultrafast Phenomena XVII*, M. Cherqui, D. M. Jonas, E. Riedle, R. W. Schoenlein, A. J. Taylor (Eds.), Oxford University Press, pp. 463 – 465 (2011)

11. T. Ebata, R. Kusaka and **S. S. Xantheas**, "Laser spectroscopic and theoretical studies of the structures and encapsulation motifs of functional molecules" in Proceedings of the International Conference of Computational Methods in Sciences and Engineering (ICCMSE-2010), Kos, Greece, *AIP Conference Proceedings* **1642**, 51 (2015)

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**D. Publications in Peer-Reviewed Scientific Journals**

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**1987**

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12. B. M. Rode and **S. S. Xantheas**, "Analysis of Energetic Effects in Lithium Fluoride Crystals by Means of *Ab-initio* and MESQUAC-MO-SCF Calculations", *Analytical Sciences* **3**, 395 (1987)

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**1990**

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13. **S. S. Xantheas**, S. T. Elbert and K. Ruedenberg, "The Potential Energy Surface of Carbon Dioxide", *Chemical Physics Letters* **166**, 39 (1990)
14. **S. Xantheas**, S. T. Elbert and K. Ruedenberg, "An Intersection Seam Between the Ground State of Ozone and an Excited State of Like Symmetry", Letter to the Editor, *Journal of Chemical Physics* **93**, 7519 (1990)

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15. P. Valtazanos, S. T. Elbert, **S. Xantheas** and K. Ruedenberg, "The Ring Opening of Cyclopropylidene to Allene: Global Features of the Reaction Surface", *Theoretica Chimica Acta* **78**, 287 (1991)
16. **S. Xantheas**, P. Valtazanos and K. Ruedenberg, "The Ring Opening of Cyclopropylidene to Allene and the Isomerization of Allene: *Ab-initio* Interpretation of the Electronic Rearrangements in Terms of Quasiatomic Orbitals", *Theoretica Chimica Acta* **78**, 327 (1991)
17. **S. Xantheas**, S. T. Elbert and K. Ruedenberg, "The Ring Opening of Cyclopropylidene to Allene: Key Features of the Accurate Reaction Surface", *Theoretica Chimica Acta* **78**, 365 (1991)
18. **S. S. Xantheas**, G. J. Atchity, S. T. Elbert and K. Ruedenberg, "Potential Energy Surfaces of Ozone. I", *Journal of Chemical Physics* **94**, 8054 (1991)
19. G. J. Atchity, **S. S. Xantheas** and K. Ruedenberg, "Potential Energy Surfaces near Intersections", *Journal of Chemical Physics* **95**, 1862 (1991)

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20. R. J. Cave, **S. S. Xantheas**, D. Feller, "Exploiting Regularity in Systematic Sequences of Wavefunctions which Approach the Full CI Limit", Klaus Ruedenberg issue (invited), *Theoretica Chimica Acta* **83**, 31 (1992)
21. **S. S. Xantheas** and T. H. Dunning, Jr., "Structures of Anion-Water Clusters:  $H^-(H_2O)_n$ ,  $n=1-3$ ", *Journal of Physical Chemistry* **96**, 7505 (1992)

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22. **S. S. Xantheas** and T. H. Dunning, Jr., "Theoretical Estimation of the Enthalpy of Formation of HSO and the HSO-SOH Isomerization Energy", *Journal of Physical Chemistry* **97**, 18 (1993)

23. **S. S. Xantheas** and T. H. Dunning, Jr., "The Structure of the Water Trimer from *Ab-initio* Calculations", *Journal of Chemical Physics* **98**, 8037 (1993)
24. **S. S. Xantheas** and T. H. Dunning, Jr., "Theoretical Studies of Sulfurous Species of Importance in Atmospheric Chemistry: I. Characterization of the HSO and SOH Isomers", *Journal of Physical Chemistry* **97**, 6616 (1993)
25. **S. S. Xantheas** and T. H. Dunning, Jr., "*Ab-initio* studies of Cyclic Water Clusters (H<sub>2</sub>O)<sub>n</sub>, n=1-6: I. Structures and Vibrational Spectra", *Journal of Chemical Physics* **99**, 8774 (1993)

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26. **S. S. Xantheas** and K. Ruedenberg, "Potential Energy Surfaces of Carbon Dioxide", Robert G. Parr issue (invited), *International Journal of Quantum Chemistry* **49**, 409 (1994)
27. **S. S. Xantheas**, "*Ab-initio* studies of the Cyclic Water Clusters (H<sub>2</sub>O)<sub>n</sub>, n=1-6: II. Analysis of Many-Body interactions", *Journal of Chemical Physics* **100**, 7523 (1994)
28. S. Deshmukh, J. D. Myers, **S. S. Xantheas**, and W. P. Hess, "Investigation of Acetyl Chloride Photodissociation by Photofragment Imaging", *Journal of Physical Chemistry* **98**, 12535 (1994)
29. **S. S. Xantheas** and T. H. Dunning, Jr., "Structures and Energetics of the F<sup>-</sup>(H<sub>2</sub>O)<sub>n</sub>, n=1-3 Clusters from *Ab-initio* Calculations", *Journal of Physical Chemistry* **98**, 13489 (1994)

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30. **S. S. Xantheas**, "*Ab-initio* studies of the Cyclic Water Clusters (H<sub>2</sub>O)<sub>n</sub>, n=1-6: III. Comparison of Density Functional with MP2 Results", *Journal of Chemical Physics* **102**, 4505 (1995)
31. **S. S. Xantheas** and T. H. Dunning, Jr., "Effect of Solvation on Chemical Reactions. I. Addition of a Single Water Molecule to the H<sup>+</sup> + H<sub>2</sub>O → OH<sup>-</sup> + H<sub>2</sub> Reaction", Y.-T. Lee issue (invited), *Journal of the Chinese Chemical Society* **42**, 241 (1995)
32. **S. S. Xantheas**, "Theoretical study of Hydroxide Ion - Water Clusters", *Journal of the American Chemical Society* **117**, 10373 (1995)
33. **S. S. Xantheas** and B. T. Sutcliffe, "The Hamiltonian for a Weakly-Interacting Trimer of Polyatomic Monomers", *Journal of Chemical Physics* **103**, 8022 (1995)

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34. **S. S. Xantheas**, "Significance of Higher Order Many-Body Interaction Energy Terms in Water Clusters and Bulk Water", *Philosophical Magazine B* **73**, 107 (1996)
35. **S. S. Xantheas** and L. X. Dang, "Critical Study of Fluoride-Water Interaction", *Journal of Physical Chemistry* **100**, 3989 (1996)
36. **S. S. Xantheas**, "On the Importance of the Fragment Relaxation Energy Terms in the Estimation of the Basis Set Superposition Error (BSSE) Correction to the Intermolecular Interaction Energy", Letter to the Editor, *Journal of Chemical Physics* **104**, 8821 (1996)
37. **S. S. Xantheas**, "Quantitative Description of Hydrogen Bonding in Chloride-Water Clusters", *Journal of Physical Chemistry* **100**, 9703 (1996)

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38. **S. S. Xantheas** and T. H. Dunning, Jr., A. Mavridis, "On the Binding Energies of NF ( $^3\Sigma^-$ ) and NCl ( $^3\Sigma^-$ )", *Journal of Chemical Physics* **106**, 3280 (1997)
39. E. Wasserman, J. R. Rustad and **S. S. Xantheas**, "Interaction Potential for Al $^{3+}$  in Water from First Principles Calculations", *Journal of Chemical Physics* **106**, 9769 (1997)
40. I. Morrison, J. C. Li and S. Jenkins, **S. S. Xantheas**, M. C. Payne, "Ab-initio Total Energy Studies of the Static and Dynamical Properties of Ice Ih", *Journal of Physical Chemistry B* **101**, 6146 (1997)
41. M. P. Hodges and A. J. Stone, **S. S. Xantheas**, "The Contribution of Many-Body Terms to the Interaction Energy of Small Water-Clusters: A Comparison of *Ab-initio* and Accurate Model Potentials", *Journal of Physical Chemistry A* **101**, 9163 (1997)

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42. **S. S. Xantheas**, G. C. Fanourgakis, S. C. Farantos and M. Velegrakis, "Spectroscopic Constants of the X- $^2\Sigma^+$  and A- $^2\Pi$  States of Sr $^+$ Ar from First Principles: Comparison with Experiment", *Journal of Chemical Physics* **108**, 46 (1998)
43. K. A. Peterson, **S. S. Xantheas**, D. A. Dixon and T. H. Dunning, Jr., "Predicting the Proton Affinities of H $_2$ O and NH $_3$ ", *Journal of Physical Chemistry A* **102**, 2449 (1998)
44. G. C. Fanourgakis, S. C. Farantos, C. Lüder, M. Velegrakis and **S. S. Xantheas**, "Photofragmentation Spectra and Structures of Sr $^+$ Ar $_n$ , n=2-8 Clusters: Experiment and Theory", *Journal of Chemical Physics* **109**, 108 (1998)
45. T. Müller, **S. S. Xantheas**, H. Dachsels, R. J. Harrison, J. Nieplocha, R. Shepard, G. Kedziora and H. Lischka, "A Systematic Ab-initio Investigation of the Open and Ring Structures of Ozone", *Chemical Physics Letters* **293**, 72 (1998)
46. E. R. Batista, **S. S. Xantheas** and H. Jónsson, "Molecular Multipole Moments of Water Molecules in Ice Ih", *Journal of Chemical Physics* **109**, 4546 (1998)
47. G. E. Froudakis, G. S. Fanourgakis and S. C. Farantos, **S. S. Xantheas**, "Binding Energies and Structures of C $^+$ Ar $_n$ , n=1-5, Clusters from First Principles", *Chemical Physics Letters* **294**, 109 (1998)
48. A. Kalemios and A. Mavridis, **S. S. Xantheas**, "Theoretical Investigation of the Ground X $^3\Sigma^-$  State of Nitrogen Bromide", *Journal of Physical Chemistry A* **102**, 10536 (1998)

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49. O. M. Cabarcos, C. J. Weinheimer, and J. M. Lisy, **S. S. Xantheas**, "Microscopic Hydration of the Fluoride Anion", Communication to the Editor, *Journal of Chemical Physics* **110**, 5 (1999)
50. C. J. Burnham and J. Li, **S. S. Xantheas**, M. Leslie, "The Parametrization of a Thole-type All-Atom Polarizable Water Model from First Principles and its Application to the Study of Water Clusters (n=2-21) and the Phonon Spectrum of Ice Ih", *Journal of Chemical Physics* **110**, 4566 (1999)
51. G. S. Fanourgakis, S. C. Farantos, Ch. Lüder, M. Velegrakis and **S. S. Xantheas**, "Photofragmentation Spectra and Potential Energy Surfaces of Sr $^+$ Ar $_2$ ", special issue of Faraday

Transactions on Chemical Reaction Theory (invited), *Physical Chemistry Chemical Physics* **1**, 977 (1999)

52. P. Weis, P. R. Kemper and M. T. Bowers, **S. S. Xantheas**, "A New Determination of the Fluoride Ion-Water Bond Energy", Communication to the Editor, *Journal of the American Chemical Society* **121**, 3531 (1999)
53. H. E. Dorsett and R. O. Watts, **S. S. Xantheas**, "Probing Temperature Effects on the Hydrogen Bonding Network of the  $\text{Cl}^-(\text{H}_2\text{O})_2$  Cluster", Letter to the Editor, *Journal of Physical Chemistry A* **103**, 3351 (1999)
54. E. R. Batista, **S. S. Xantheas**, H. Jónsson "Multipole Moments of Water Molecules in Clusters and Ice Ih from First Principles Calculations", *Journal of Chemical Physics* **111**, 6011 (1999)
57. P. Ayotte, S. B. Nielsen, G. H. Weddle, and M. A. Johnson, **S. S. Xantheas** "Spectroscopic observation of ion-induced water dimer dissociation in the  $\text{X}^-(\text{H}_2\text{O})_2$  ( $\text{X}=\text{F}, \text{Cl}, \text{Br}, \text{I}$ ) clusters", Letter to the Editor, *Journal of Physical Chemistry A* **103**, 10665 (1999)

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56. E. R. Batista, **S. S. Xantheas**, H. Jónsson "Electric Fields in Ice and Near Water Clusters", *Journal of Chemical Physics* **112**, 3285 (2000). Featured in the *Virtual Journal of Biological Physics Research*
57. D. Tzeli, A. Mavridis and **S. S. Xantheas** "A First Principles Study of the Microhydration of Acetylene", *Journal of Chemical Physics* **112**, 6178 (2000)
58. T. A. Blake, S. W. Sharpe and **S. S. Xantheas** "Rotationally Resolved Spectroscopy of a Librational Fundamental Band of Hydrogen Fluoride Tetramer", *Journal of Chemical Physics* **113**, 707 (2000)
59. **S. S. Xantheas**, "Cooperativity and Hydrogen Bonding Network", special issue on Water (invited), *Chemical Physics* **258**, 225 (2000)

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60. D. Tzeli and A. Mavridis, **S. S. Xantheas**, "A molecular level study of the aqueous microsolvation of acetylene", *Chemical Physics Letters* **340**, 538 (2001)

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61. C. J. Burnham and **S. S. Xantheas**, "Development of Transferable Interaction Potentials for Water: I. Prominent Features of the Water Dimer Potential Energy Surface", *Journal of Chemical Physics* **116**, 1479 (2002). Featured in the *Virtual Journal of Biological Physics Research*
62. **S. S. Xantheas**, C. J. Burnham, R. J. Harrison, "Development of Transferable Interaction Potentials for Water: II. Accurate Energetics of the First Few Water Clusters from First Principles", *Journal of Chemical Physics* **116**, 1493 (2002). Featured in the *Virtual Journal of Biological Physics Research*
63. C. J. Burnham and **S. S. Xantheas**, "Development of Transferable Interaction Potentials for Water: III. Re-parameterization of an All-Atom Polarizable Rigid Model (TTM2-R) from First Principles", *Journal of Chemical Physics* **116**, 1500 (2002)
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65. T. H. Dunning, Jr., R. J. Harrison, D. Feller, and **S. S. Xantheas**, "Promise and Challenge of High-performance Computing, with Examples from Molecular Modeling", special issue on "New Science from High Performance Computing" (invited), *Philosophical Transactions of the Royal Society of London, Series A, Mathematical and Physical Sciences* **360**, 1079 (2002)
66. C. J. Burnham and **S. S. Xantheas**, M. A. Miller, B. Applegate and R. E. Miller, "The Formation of Cyclic Water Complexes by Sequential Ring Insertion: Experiment and Theory", *Journal of Chemical Physics* **117**, 1109 (2002)
67. P. R. McCurdy, W. P. Hess and **S. S. Xantheas**, "Nitric Acid-Water Complexes: Theoretical Calculations and comparison with Experiment", G. Wilse Robinson Festschrift (invited), *Journal of Physical Chemistry A* **106**, 7628 (2002)
68. D. Tzeli and A. Mavridis, **S. S. Xantheas**, "A First Principles Examination of the Acetylene-Water clusters, HCCH-(H<sub>2</sub>O)<sub>n</sub>, n=2, 3 and 4", *Journal of Physical Chemistry A* **106**, 11327 (2002)

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69. G. M. Chaban, **S. S. Xantheas**, R. B. Gerber, "Anharmonic Vibrational Spectroscopy of the F<sup>-</sup>(H<sub>2</sub>O)<sub>n</sub> complexes, n=1, 2", *Journal of Physical Chemistry A* **107**, 4952 (2003)

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70. **S. S. Xantheas**, E. Aprà, "The binding energies of the D<sub>2d</sub> and S<sub>4</sub> water octamer isomers: High-level electronic structure and empirical potential results", *Journal of Chemical Physics* **120**, 823 (2004). Featured in the *Virtual Journal of Biological Physics Research*
71. J. M. Bowman, **S. S. Xantheas**, "Morphing of *ab initio*-based interaction potentials to spectroscopic accuracy: Application to Cl<sup>-</sup>(H<sub>2</sub>O)", *Pure and Applied Chemistry* **76**, 29 (2004)
72. C. J. Burnham and **S. S. Xantheas**, "On the importance of zero-point effects in molecular level classical simulations of water", *Journal of Molecular Liquids* **110**, 177 (2004)
73. G. S. Fanourgakis, E. Aprà and **S. S. Xantheas**, "High-level *ab-initio* calculations for the four low-lying families of minima of (H<sub>2</sub>O)<sub>20</sub>: I. Estimates of MP2/CBS binding energies and comparison with empirical potentials", *Journal of Chemical Physics* **121**, 2655 (2004)

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