FRANCESCO PAESANI

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EDUCATION

2000	Ph.D. Theoretical Physical Chemistry Department of Chemistry University of Rome "La Sapienza" (Italy) Thesis: "Van der Waals Interactions from Density Functional Methods: A Theoretical Study and Dynamical Calculations" Advisor: Professor F.A. Gianturco
1996	Laurea, Summa cum Laude Department of Chemistry University of Rome "La Sapienza" (Italy) Thesis: "Van der Waals Interactions from Density Functional Methods: Vibrational relaxation in the He-CO system" Advisor: Professor F.A. Gianturco

PROFESSIONAL EXPERIENCE

07/2017 – Present	Professor Department of Chemistry and Biochemistry University of California, San Diego
07/2015 – 06/2017	Associate Professor Department of Chemistry and Biochemistry University of California, San Diego
07/2009 – 06/2015	Assistant Professor Department of Chemistry and Biochemistry University of California, San Diego
2001	Lecturer Department of Chemistry University of Rome "La Sapienza" (Italy)

RESEARCH EXPERIENCE

2005 – 2009	Postdoctoral Research Fellow in the group of Professor G.A. Voth Department of Chemistry, University of Utah, Salt Lake City

- Principal developer of the AMBER code (http://ambermd.org)
- Developed and applied Multi State Empirical Valence (MS-EVB) methods for proton transfer and transport in condensed phase systems
- Developed and applied quantum methods for simulations of aqueous systems using *ab initio*-based and polarizable force fields

2002 – 2005 Postdoctoral Associate in the group of Professor K.B. Whaley
Department of Chemistry, University of California, Berkeley

- Developed and applied quantum methods for characterizing molecular clusters

1997 – 2000 Graduate Research Assistant
Department of Chemistry, University of Rome "La Sapienza"
Advisor: Professor F.A. Gianturco

- Developed density functional theory methods for non-bonded interactions

HONORS AND AWARDS

2017	UC San Diego Legacy Lecture
2016	ACS Early Career Award in Theoretical Chemistry
2016	UC San Diego Office for Students with Disabilities Award of Recognition
2015	NSF CAREER
2014	ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry
2012	Hellman Fellowship
1997 – 2000	Departmental Graduate Fellowship in Theoretical Physical Chemistry University of Rome "La Sapienza" (Italy)
1991 – 1996	Departmental Undergraduate Scholarship in Chemistry University of Rome "La Sapienza" (Italy)

PROFESSIONAL AFFILIATIONS

American Chemical Society

American Physical Society

TEACHING EXPERIENCE

University of California, San Diego

Chem 6BH: Honors General Chemistry II (2013-2017)

Chem 126: Physical Chemistry: Quantum Mechanics (2015-2016)

Chem 131: Chemical Physics: Stat Thermo (2011-2013)

Chem 185/285: Introduction to Computational Chemistry (2010-2012)

University of Rome "La Sapienza" (Italy)

Physical Chemistry (2001)

Physical Chemistry (Lab instructor, 1994-1996)

POSTDOCTORAL RESEARCHERS SUPERVISED

Volodymyr Babin (2011-2013), Kyoyeon Park (2011-2013), Jordi Cirera (2011-2014), Anthony Clark (2013-2014), Zack Terranova (2014-2015), Chungwen Liang (2014-2015), Gianmarc Grazioli (2016), Santosh Meena (2016), Daniel Moberg (2015-present), Sandeep Reddy (2015-present), Huy Pham (2015-present), Sandra Brown (2016-present).

GRADUATE STUDENTS SUPERVISED

Jason Grosch (M.S. 2011), Jeffrey Sung (M.S. 2012), Wei Lin (Ph. D. 2014), Greg Medders (Ph. D. 2015), Pushp Bajaj (Ph. D. current), Shelby Straight (Ph. D. current), Marc Riera (Ph. D. current), Colin Egan (Ph. D. current), Oliver Hamto (Ph. D. current).

UNDERGRADUATE STUDENTS SUPERVISED

Allen Chan (2009-2010), Nico Sawaya (2009-2011), Porter Howland (2012), Kevin Bao (2012-2013), Blake Tsu (2012-2013), Matt Agee (2013-2014), Ximin Chen (2013-2014), Danica Moore (2012-2013), Jason Wong (2013-2014), Adil Mohd-Salleh (2013-2014), Yu Fan (2013-2014), David Sanchez (2013-2015), Jiarong Zhou (2014-2016), Matt Hung (2015-2016), Carolyn White (2015-2016), Sebastian Amara (2015-2016), Minyue Fan (2016), Karl Chen (2016), Debbie Zhuang (2016-present), Zhonghuan Luo (2016-present), Qin Li (2017-present), Eric Yeh (2017-present).

UNIVERSITY AND DEPARTMENT SERVICE

- UC San Diego: Department of Chemistry and Biochemistry, Graduate Admissions and Recruitment Committee (2010 – 2013, 2014 – present)
- UC San Diego: Department of Chemistry and Biochemistry, Physical Chemistry First Year Graduate Advisor (2009 – 2011, 2013 – 2014)
- UC San Diego: Department of Chemistry and Biochemistry, Research Computing Committee (2009 – 2011)
- UC San Diego: Department of Chemistry and Biochemistry, Physical Chemistry Seminar Committee (2010 – 2013)
- UC San Diego: Chemistry and Biochemistry liaison for the Study Abroad Program (2012 –

present)

CONTRACTS AND GRANTS

CURRENT

- NSF CHE-1038028 (Center for Chemical Innovation, Co-I, 09/01/2013 – 08/31/2018)
- AFOSR FA9550-16-1-0327 (PI, 08/15/2016 – 08/14/2019)
- ARO W911NF-15-1-0189 (Co-PI, 07/01/2015 – 06/30/2018)
- NSF CAREER CHE-1453204 (PI, 04/01/2015 – 03/31/2020)
- NSF ACI-1642336 (PI, 04/01/2017 – 03/31/2020)
- XSEDE: 3,291,831 SUs on the NSF supported Gordon computing cluster, 4,489,704 SUs on the NSF supported Comet computing cluster, 552,960 SUs on the NSF supported Maverick Interactive Visualization and Data Analytics System (PI, 04/01/2016 – 03/31/2017)

COMPLETED

- DOE DE-FG02-13ER16387 (PI, 06/01/2013 – 11/30/2016)
- UC San Diego, Integrated Digital Infrastructure (PI, 10/01/2015 – 09/30/2016)
- UC San Diego, Frontiers of Innovation Scholars Program (PI, 01/01/2016 – 31/01/2016)
- NSF DMR-1305101 (PI, 09/01/2013 – 08/31/2016)
- NSF CHE-1111364 (PI, 08/015/2011 – 08/14/2014)
- Triton Research Opportunities, UC San Diego (PI, 2011)
- TERAGRID 1,000,000 SUs on the NSF supported Trestles computing cluster (PI, 01/01/2012 – 12/31/2013)
- XSEDE: 4,438,743 SUs on the NSF supported Trestles and Gordon computing clusters (PI, 01/01/2013 – 12/31/2012)
- XSEDE: 8,237,728 SUs on the NSF supported Trestles and Gordon computing clusters, 468,316 SUs on the NSF supported Maverick Interactive Visualization and Data Analytics System, and 1TB of data storage (PI, 04/01/2015 – 03/31/2016)
- XSEDE: 4,300,807 SUs on the NSF supported Gordon computing cluster, 1,600,000 SUs on the NSF supported Comet computing cluster, 552,960 SUs on the NSF supported Maverick Interactive Visualization and Data Analytics System (PI, 04/01/2015 – 03/31/2016)

EDITORIAL ACTIVITIES

- Member of the Editorial Advisory Board for The Journal of Physical Chemistry.
- Reviewer for Accounts of Chemical Research, Angewandte Chemie International Edition, ChemPhysChem, Chemical Physical Letters, Chemical Science, Journal of Chemical Physics, Journal of Low Temperature Physics, Journal of Physical Chemistry (A, B, C and Letters), Journal of the American Chemical Society, Journal of Chemical Theory and Computation, Molecular Simulation, Nano Letters, Nature Chemistry, Nature

Communications, Physical Chemistry Chemical Physics, Proceedings of the National Academy of Sciences U.S.A., Science, Structural Dynamics.

- Reviewer for the National Science Foundation, Department of Energy, and Department of Defense.

SCIENTIFIC SOFTWARE DEVELOPMENT

- AMBER suite of codes for molecular simulations (http://ambermd.org)
- MB-pol plugin (http://paesanigroup.ucsd.edu/software/mbpol_openmm.html) for OpenMM (https://simtk.org/home/openmm)
- MB-pol interface (http://paesanigroup.ucsd.edu/software/mbpol_ipi.html) for the i-PI wrapper for molecular simulations (https://github.com/i-pi/i-pi)

OUTREACH ACTIVITIES

- Chair Elect for the Theoretical Chemistry Subdivision of the American Chemical Society.
- Member of the Editorial Advisory Board for the Journal of Physical Chemistry (2017 – 2019).
- UC San Diego, Summer Training Academy for Research Success (STARS) program for community college students, undergraduate students, recent graduates and masters students.
- UC San Diego, Research Scholars Program for high school students.

CONFERENCES AND SEMINARS

Invited talks

1. *XIX International Symposium on Molecular Beams*, June 3 - 8, 2001, Rome (Italy)
   "Structure and dynamics of OCS impurity in helium clusters"
2. *ACS National Meeting*, September 7 - 11, 2003, New York (NY)
   "Direct calculation of excited state energies by spectral evolution Monte Carlo"
3. *Doped Rare Gas Clusters*, June 24 - 30, 2002, Telluride (CO)
   “Rotational excitations in doped helium clusters”
4. *Gordon Research Conference “Vibrational Spectroscopy”*, July 11 - 16, 2004, Bristol (RI)
   "Vibrational spectroscopy of OCS and OCS complexes with H_2 in He clusters”
5. *ACS National Meeting*, August 22 - 26, 2004, Philadelphia (PA)
   “Superfluid solvation in helium and para-hydrogen clusters”
6. *Pacifichem 2005*, December 15 - 20, 2005, Honolulu (HI)
   “Recent advances for condensed phase quantum dynamics”
7. *Physical Chemistry Seminar*, February 12, 2008, UC San Diego (CA)
   “Rethinking water: do we really understand it and can we model it accurately?”
8. *Theoretical Chemistry Seminar*, June 5, 2008, Leiden University, Leiden (Netherlands)
   “Nuclear quantum effects are important for the properties of water and ice”
9. *Aqueous Solutions and their Interfaces*, June 23 - 27, 2008, Crete (Gr)
   “Is nuclear quantization important to understand the behavior of water?”

10. *Physical Chemistry Seminar*, November 17, 2008, University of Alberta, Edmonton (AB)
"Understanding condensed-phase phenomena through quantum molecular dynamics"
11. *Physical Chemistry Seminar*, December 4, 2008, Cornell University, Ithaca (NY)
"Understanding condensed-phase phenomena through quantum molecular dynamics"
12. *Physical Chemistry Seminar*, December 8, 2008, UC Merced (CA)
"Understanding condensed-phase phenomena through quantum molecular dynamics"
13. *Physical Chemistry Seminar*, January 8, 2009, Wayne State University (MI)
"Understanding condensed-phase phenomena through quantum molecular dynamics"
14. *Physical Chemistry Seminar*, January 14, 2009, University of Virginia (VA)
"Understanding condensed-phase phenomena through quantum molecular dynamics"
15. *Physical Chemistry Seminar*, February 19, 2009, UC San Diego (CA)
"Understanding condensed-phase phenomena through quantum molecular dynamics"
16. *Chemical & Materials Sciences Seminar,* May 28, 2009, Pacific Northwest National Laboratory, Richland (WA)
"The properties of water: Insights from quantum simulations"
17. TSRC Workshop on *Electrification of Water Drops and Ice Particles: Through Simulations, in the Laboratory and in the Natural Environment.* August 10 - 14, 2009, Telluride (CO)
"The properties of water and ice surfaces"
18. *Physical Chemistry Seminar*, April 5, 2010, University of Southern California (CA)
"Computational spectroscopy: Linking structural and dynamical properties in the condensed phase"
19. CECAM workshop on *Advances in the implementation of polarizable force fields for molecular simulations*, June 7 - 9, 2010, Lausanne (Switzerland)
"Infrared spectroscopy of aqueous systems from quantum simulations with the TTM3-F polarizable model"
20. TSRC Workshop on *Condensed Phase Dynamics,* July 19 - 23, 2010, Telluride (CO)
"Computational spectroscopy of water: Linking structural and dynamical properties"
21. *Physical Chemistry Seminar,* October 5, 2010, California State University, Los Angeles
"Towards a first principles description of aqueous environments"
22. CECAM Workshop on *Liquid/solid interfaces: Structure and dynamics from spectroscopy and simulation",* June 27 - 29, 2011, Lausanne (Switzerland)
"Water in cavity-ligand binding: Structure, dynamics and spectroscopic signatures"
23. *ACS National Meeting,* August 28 - September 1, 2011, Denver (CO)
"Molecular-level modeling of heterogeneous chemistry on aerosol surfaces"
24. *Physical Chemistry Seminar,* October 31, 2011, University of Utah, Salt Lake City (UT)
"The properties of water and ice: Insights from quantum molecular dynamics simulations"
25. *Theoretical Chemistry Institute Seminar,* March 5, 2012, University of Wisconsin, Madison (WI)
"Molecular-level modeling of metal-organic frameworks: Breathing, adsorption, and quantum effects"
26. *ACS National Meeting,* March 25-29, 2012, San Diego (CA)

"Computational studies of heterogeneous chemistry at ice surfaces"

27. *Computational Chemistry Seminar,* June 13, 2012, UC Irvine (CA)
"Nuclear quantum effects in water: From clusters to bulk".

28. TSRC Workshop on *Condensed Phase Dynamics,* June 26 - 29, 2012, Telluride (CO)
"Water models and simulations"

29. *ACS National Meeting,* August 19 - 23, 2012, Philadelphia (PA)
"Water in cavity-ligand binding: Structure, dynamics, and spectroscopic signatures"

30. *ACS National Meeting,* August 19 - 23, 2012, Philadelphia (PA)
"Heterogeneous chemistry on aerosols: Molecular-level modeling and simulation"

31. *ACS National Meeting,* August 19 - 23, 2012, Philadelphia (PA)
"Computational studies of aerosol surfaces"

32. *Physical Chemistry Seminar,* April 18, 2013, University of South Florida, Tampa (FL)
"Molecular-level modeling of MOFs: Breathing, water adsorption, and proton conduction"

33. TSRC Workshop on *Quantum Effects in Condensed-Phase Systems,* July 8 - 12, 2013, Telluride (CO)
"The curious case of the water hexamer: Mr. Cage vs. Mr. Prism"

34. TSRC Workshop on *Intermolecular Interactions: New Challenges for Ab Initio Theory,* July 15 - 19, 2013, Telluride (CO)
"Potential problems with water simulations: From the dimer to the liquid at the fully quantum-mechanical level"

35. 12th Annual Mercury Conference on Undergraduate Computational Chemistry, July 25 - 27, 2013, Bucknell University, Lewisburg (PA)
"Molecular-level modeling of MOFs: Breathing, water adsorption, and proton conduction"

36. *ACS National Meeting,* September 8 - 13, 2013, Indianapolis (IN)
"Quantum simulations of water on a CCSD(T)-level potential: From the gas to the condensed phase"

37. *Physical Chemistry Seminar,* October 11, 2013, UC Merced (CA)
"Molecular-level modeling of MOFs: Breathing, water adsorption, and proton conduction"

38. *Physical Chemistry Seminar,* November 8, 2013, California Institute of Technology, Pasadena (CA)
"Molecular-level modeling of MOFs: Breathing, proton conduction, and spin crossover"

39. *Nanoengineering Seminar,* November 20, 2013, UC San Diego (CA)
"Molecular-level modeling of multifunctional MOFs: Breathing, proton conduction, and spin crossover"

40. *Physical Chemistry Seminar,* February 11, 2014, Northwestern University, Evanston (IL)
"Computer modeling of metal-organic frameworks: From molecular adsorption to proton conduction"

41. *Physical Chemistry Seminar,* February 12, 2014, The University of Chicago, Chicago (IL)
"Coarse graining electrons: Many-body potentials with chemical accuracy for condensed phase simulations"

42. *Physical Chemistry Seminar,* February 13, 2014, University of Illinois, Urbana-Champaign (IL)

"Computer modeling of metal-organic frameworks: From molecular adsorption to proton conduction"

43. *APS National Meeting,* March 3 - 7, 2014, Denver (CO)
"Water adsorption and proton conduction in metal-organic frameworks: Insights from molecular simulations"

44. *Physical Chemistry Seminar,* April 4, 2014, University of Colorado, Boulder (CO)
"Computer modeling of metal-organic frameworks: From molecular adsorption to proton conduction"

45. *Physical Chemistry Seminar,* April 14, 2014, The Ohio State University, Columbus (OH)
"Coarse graining electrons: Many-body water potential with chemical accuracy for condensed phase simulations"

46. *Physical Chemistry Seminar,* April 21, 2014, University of Southern California, (CA)
"Computer modeling of metal-organic frameworks: From molecular adsorption to proton conduction"

47. *Physical Chemistry Seminar,* April 24, 2014, University of Pittsburgh, Pittsburgh (PA)
"Coarse graining electrons: Many-body potentials with chemical accuracy for condensed phase simulations"

48. *Physical Chemistry Seminar,* April 30, 2014, UC Davis (CA)
"Computer modeling of metal-organic frameworks: From molecular adsorption to proton conduction"

49. *Physical Chemistry Seminar,* May 5, 2014, Stanford University, Stanford (CA)
"Computer modeling of metal-organic frameworks: From molecular adsorption to proton conduction"

50. *225th ECS Meeting,* May 11 - 16, 2014, Orlando (FL)
"Proton conduction in metal-organic frameworks: Insights from molecular dynamics simulations"

51. TSRC Workshop on *Nonlinear optics at interfaces,* June 9 - 13, 2014, Telluride (CO)
"From molecular interactions to spectroscopy: A (possible) new route to SFG"

52. TSRC Workshop on *Many-body interactions: From quantum mechanics to force fields,* June 15 - 19, 2014, Telluride (CO)
"Water potential with chemical accuracy for simulations from the gas to the condensed phase"

53. TSRC Workshop on *Condensed phase dynamics,* June 24 - 28, 2014, Telluride (CO)
"Computer modeling of metal-organic frameworks: From molecular adsorption to spin crossover"

54. TSRC Workshop on *Metal-organic frameworks: Experiments and simulations,* July 7 - 11, 2014, Telluride (CO)
"Water dynamics and proton transport in MOFs"

55. TSRC Workshop on *Spectroscopy and dynamics of coupled anharmonic vibrations of floppy molecular systems,* July 14 - 18, 2014, Telluride (CO)
"Vibrational spectroscopy of water in metal-organic frameworks"

56. Gordon Research Conference *Water and aqueous solutions,* July 27 – August 1, 2014, Holderness (NH)
"Coarse-graining electrons: Many-body water potential with chemical accuracy for

simulations from clusters to interfaces"

57. *ACS National Meeting,* August 10 - 14, 2014, San Francisco (CA)
"Computational modeling of aerosol surfaces"

58. *ACS National Meeting,* August 10 - 14, 2014, San Francisco (CA)
"Molecular dynamics simulations of catalytic metal-organic frameworks"

59. *ACS National Meeting,* August 10 - 14, 2014, San Francisco (CA)
"Proton conduction in metal-organic frameworks: Insights from molecular simulations"

60. *Water – The Most Anomalous Liquid,* October 20 - 24, 2014, Stockholm (Sweden)
"Coarse graining electrons: Many-body water potential for simulations from the gas to the condensed phase"

61. *Physical Chemistry Seminar,* November 7, 2014, Columbia University, New York City (NY)
"Coarse-graining electrons: Many-body potentials with chemical accuracy for condensed-phase simulations and vibrational spectroscopy"

62. *Gordon Research Conference "Gaseous Ions: Structures, Energetics, and Reactions",* February 22 - 27, 2015, Galveston (TX)
"Computer modeling of hydration phenomena: From clusters to bulk"

63. *Machine Learning for Many-Particle Systems,* February 23 - 27, 2015, Los Angeles (CA)
"Many-body molecular dynamics for chemically accurate simulations from the gas to the condensed phase"

64. *ACS National Meeting,* March 22- 26, 2015, Denver (CO)
"New computational tools for modeling metal-organic frameworks"

65. Workshop on *Dynamical Quantum Effects in Molecular Processes,* May 14, 2015, New York City (NY)
"Vibrational spectroscopy of water from quantum many-body molecular dynamics"

66. TSRC Workshop on *Metal-Organic Frameworks: Experiments and Simulations,* June 14 - 18, 2015, Telluride (CO)
"New computational tools for modeling metal-organic frameworks"

67. *Dynamics of Molecular Collisions,* July 12 -17, 2015, Asilomar (CA)
"Many-body molecular dynamics: A first principles approach to vibrational spectroscopy in the condensed phase"

68. TSRC Workshop on *Quantum Effects in Condensed-Phase Systems,* July 20 - 24, 2015, Telluride (CO)
"Molecular simulations of water and beyond: We fixed the interactions (yes, we did!), what about the quantum dynamics?"

69. *Physical Chemistry Seminar,* September 11, 2015, Rutgers University – Newark (NJ)
"Many-body molecular dynamics: Towards spectroscopically accurate molecular simulations in the condensed phase"

70. *Theoretical Chemistry Seminar,* September 29, 2015, Ecole Normale Supérieure – Paris (France)
"Vibrational spectroscopy of water from (quantum) many-body molecular dynamics"

71. *Theoretical Chemistry Seminar,* September 30, 2015, Université de Evry – Evry (France)
"Many-body approaches for chemically accurate molecular simulations of aqueous systems"

72. *Theoretical Chemistry Seminar,* October 2, 2015, ETH – Zurich (Switzerland)
"Many-body molecular dynamics: Towards chemically and spectroscopically accurate molecular simulations from the gas to the condensed phase"

73. Workshop on *Water at the Interface between Biology, Chemistry, Physics and Materials Sciences*, October 5 – 9, 2015, Trieste (Italy)
"By chance or by design? Towards a spectroscopically accurate ab-initio water potential from the gas to the condensed phase"

74. *Physical Chemistry Seminar*, November 24, 2015, UC Irvine (CA)
"Many-body molecular dynamics: Towards chemically and spectroscopically accurate molecular simulations from the gas to the condensed phase"

75. *Pacifichem,* December 15 - 18, 2015, Honolulu (HI)
"First principles vibrational spectroscopy of water from many-body molecular dynamics"

76. *ACS National Meeting,* March 13- 17, 2016, San Diego (CA)
"Many-body molecular dynamics: Towards chemically accurate molecular simulations from the gas to the condensed phase"

77. *ACS National Meeting,* March 13- 17, 2016, San Diego (CA)
"Dissecting the molecular structure of the air/water interface from many-body simulations of sum-frequency generation spectra"

78. *ACS National Meeting,* March 13- 17, 2016, San Diego (CA)
"Many-body molecular dynamics: An accurate approach to vibrational spectroscopy of water at complex interfaces"

79. *CPMD 2016,* May 18- 26, 2016, Chicago (IL)
"Many-body potentials for molecular simulations from the gas to the condensed phase"

80. TSRC Workshop on *Nonlinear Optics at Interfaces,* June 21 -25, 2016, Telluride (CO)
"Quantum simulations of the SFG spectrum of the air/water interface"

81. TSRC Workshop on *Condensed phase dynamics,* June 27 – July 1, 2016, Telluride (CO)
"Spin crossover in metal-organic frameworks"

82. Gordon Research Conference *Molecular Interactions & Dynamics,* July 10 – 15, 2016, Stonehill College, Easton (MA)
"Many-Body Molecular Dynamics: A New Methodology for Computer Simulations with Chemical and Spectroscopic Accuracy of Aqueous Systems from the Gas to the Condensed Phase"

83. Gordon Research Conference *Vibrational Spectroscopy,* July 17 – 22, 2016, University of New England, Biddeford (MA)
"Dissecting vibrational spectra from many-body molecular dynamics simulations"

84. Gordon Research Conference *Water & Aqueous Solutions,* July 31 – August 5, 2016, Holderness School, Holderness (NH)
Discussion Leader. "Water properties from fundamental studies"

85. *ACS National Meeting,* August 21 – 25, 2016, Philadelphia (PA)
"Many-body potential energy surfaces with chemical and spectroscopic accuracy"

86. *MOF 2016,* September 11 – 15, 2016, Long Beach (CA)
"Proton conduction in metal-organic frameworks: Insights from molecular dynamics simulations"

87. *Physical Chemistry Seminar*, September 27, 2016, Yale University, New Haven (CT)

"Achieving chemical and spectroscopic accuracy from the gas to the condensed phase from many-body representations"

88. *4th International Conference on Molecular Simulation,* October 23 – 26, 2016, Sendai (China)
"Many-body molecular dynamics: Chemical and spectroscopic accuracy from the gas to the condensed phase"

89. *Physical Chemistry Seminar*, November 6, 2016, Temple University, Philadelphia (PA)
"Understanding hydration, one water molecule at a time"

90. *Physical Chemistry Seminar*, December 6, 2016, Georgia Tech, Atlanta (GA)
"Many-body molecular dynamics: Chemical and spectroscopic accuracy, one molecule at a time"

91. *Physical Chemistry Seminar*, March 7, 2017, UC Berkeley, Berkeley (CA)
"Understanding hydration, one water molecule at a time"

92. *APS National Meeting,* March 13 – 17, 2017, New Orleans (LA)
"Many-Body Molecular Dynamics: Chemical and Spectroscopic Accuracy from the Gas to the Condensed Phase"

93. *ACS National Meeting,* April 2 – 6, 2017, San Francisco (CA)
"Dissecting the molecular structure and dynamics of aqueous systems through many-body molecular dynamics simulations"

94. *Physical Chemistry Seminar*, April 28, 2017, Penn State University, University Park (PA)
"Understanding hydration, one water molecule at a time"

95. *Physical Chemistry Seminar*, April 26, 2017, University of North Carolina - Chapel Hill
"Understanding hydration, one water molecule at a time"

96. *9th International Conference on Advanced Vibrational Spectroscopy*, June 11 – 16, Victoria (BC), Canada
"Infrared spectroscopy from many-body molecular dynamics"

97. *American Conference on Theoretical Chemistry*, July 16 – 21, Boston (MA)
"Chemical accuracy from the gas to the condensed phase through many-body molecular dynamics"

Contributed talks

1. *Complex Systems: Structure, Reactivity and Dynamics*, June 16 – 18, 1999, Varenna (Italy)
"Solvation model for simple molecules: A DFT and DMC study for $CO(Rg)_N$ solutions"

2. *California Helium Studies Group Meeting*, May 4, 2002, University of Southern California, Los Angeles (CA)
"Rotational excitations of the OCS molecule in ^{4}He clusters"

3. *Doped Rare Gas Clusters,* June 24 – 30, 2002, Telluride (CO)
"Rotational excitations in doped helium clusters"

4. *California HeII Third Annual Workshop*, May 17, 2003, Berkeley (CA)
"OCS in small para-hydrogen clusters"

5. *International Symposium on Molecular Spectroscopy*, June 20 – 24, 2005, Columbus (OH), "Rotational spectra of molecules in small He clusters: Probing superfluidity in finite

systems”

6. *ACS National Meeting*, August 19 – 23, 2007, Boston (MA)
   “Nuclear quantum effects: A key factor for water structure and dynamics?”
7. *ACS National Meeting*, March 22 – 26, 2009, Salt Lake City (UT)
   “Hydrogen-bond dynamics in liquid water from an ab initio-based polarizable force field”
8. *ACS National Meeting,* August 22 – 26, 2010, Boston (MA)
   “The properties of the ice surface from quantum molecular dynamics simulations”
9. *ACS National Meeting,* March 25 – 29, 2012, San Diego (CA)
   “Water structure, dynamics and spectroscopy in metal-organic frameworks”
10. *ACS National Meeting,* April 7 – 11, 2013, New Orleans (LO)
    “Toward a universal water model: From the dimer to the liquid phase at the CCSD(T) level”
11. *ACS National Meeting,* March 16 – 21, 2014, Dallas (TX)
    “Water potential from first principles”
12. *ACS National Meeting,* March 16 – 21, 2014, Dallas (TX)
    “Molecular modeling of proton conduction in metal-organic frameworks”
13. *ACS National Meeting,* August 10 – 14, 2014, San Francisco (CA)
    “Coarse graining electrons: Many-body potentials with chemical accuracy for condensed phase simulations”
14. *MOF2014, 4th International Conference on Metal-Organic Framework and Open Framework Compounds,* September 28 – October 1, 2014, Kobe (Japan)
    “Computer modeling of metal-organic frameworks: From water adsorption to proton conduction”
15. *Pacifichem,* December 15 – 18, 2015, Honolulu (HI)
    “Ab initio many-body potentials for chemically accurate simulations from the gas to the condensed phase”; “Computer modeling of proton conduction in metal-organic frameworks”

Poster Sessions

1. *XIX National Conference of Atomic and Molecular Physics*, October 23 – 26, 1996, Perugia (Italy)
   "Vibrational relaxation in He-CO mixtures: Dynamics and interaction forces"
2. *CCP6 Workshop "Fashioning a model: optimization methods in chemical physics"*, March 24 – 27, 1998, Durham (UK)
   "The use of DFT methods for calculation of van der Waals interactions in molecular systems”
3. *ECAMP VI - The Sixth European Conference on Atomic and Molecular Physics*
   July 14 – 18, 1998, Siena (Italy)
   "The use of DFT methods for the calculation of van der Waals interactions: Computed and measured transport coefficients for rare gas-molecule mixtures"
4. *MOLEC XII - The Twelfth European Conference on Dynamics of Molecular Collisions*
   September 6 – 11, 1998, Bristol (UK)
   "Solvation model for simple molecules: a DFT and DMC study for $CO(He)_N$ and $CO(Ar)_N$

clusters"

5. *Gordon Research Conference "Molecular and Ionic Clusters"*, April 16 – 21, 2000, Toulouse (France)
"Diffusion Monte Carlo calculations for $OCS(He)_N$ clusters: Structures and energetics"
6. *MOLEC 2000 - The XIIIth European Conference on Dynamics of Molecular Collisions*, September 17 – 22, 2000, Jerusalem (Israel)
"Diffusion Monte Carlo calculations for $OCS(He)_N$ clusters: Structures and energetics"
7. *Faraday Discussion 118 "Cluster Dynamics"*, April 18 – 20, 2001, Durham, (UK)
"Structure and dynamics of OCS impurity in helium clusters"
8. *INFMeeting National Conference on Physics Matter*, June 18 – 22, 2001, Rome (Italy)
"Molecular impurities in ^{4}He as probes of nanoscopic superfluidity"
9. *XIXth Conference on the Dynamics of Molecular Collisions*, July 13 – 18, 2003, Lake Tahoe (CA)
"OCS in small para-hydrogen clusters: Energetics, structures and superfluidity"
10. *QFS 2003*, August 3 – 8, 2003, Albuquerque (NM)
"Superfluid solvation of OCS in ^{4}He and pH_2 clusters"
11. *Advances in Computational Many-Body Physics*, January 13 – 16, 2005, Banff (Alberta)
“OCS in para-hydrogen and mixed helium/para-hydrogen clusters: energetics, structures and superfluidity”
12. *47th Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory*, February 22 – 27, 2007, St. Simons Island (GA)
“A quantitative analysis of quantum effects in liquid water”

Schools and Professional Workshops

1. Scuola Nazionale di Fisica Atomica e Molecolare: recenti sviluppi ed applicazioni
November 4 – 10, 1996, Trento (Italy)
2. Gaussian Workshop
April 21 – 24, 1998, Rome (Italy)
3. Amber Developers meeting
October 26 – 29, 2005, Salt Lake City (UT)
4. Amber Developers meeting
February 22 – 27, 2007, St. Simons Island (GA)
5. Amber Developers meeting
October 19 – 22, 2007, La Jolla (CA)
6. Amber Developers meeting
February 27 – March 2, 2009, St. Simons Island (GA)
7. Workshop on *Path to Petascale: Adapting GEO/CHEM/ASTRO Applications for Accelerators and Accelerator Clusters*
April 1 – 3, 2009, Urbana (IL)
8. *Amber Developers meeting*
January 21 – 23, 2010, Stony Brook (NY)

LIST OF PUBLICATIONS

Articles published in peer-reviewed journals

* At this time it was a standard in Prof. Gianturco's lab to follow the alphabetical order. I served as the lead contributor for the theoretical part of these studies.

1. F.A. Gianturco*, F. Paesani, M.F. Laranjeira, V. Vassilenko, M.A. Cunha, A.G. Shashkov, A.F. Zolotoukhina, "Computed and measured thermal diffusion factor for CO-He mixtures: a test of recent potentials", *Mol. Phys.* 92, 957 (1997).
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Book chapters

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