Paolo Carloni

Curriculum Vitae

December, 2012

PERSONAL DATA

Office address:
German Research School for Simulation Sciences GmbH, Jülich, Germany
Tel +49 2461 61-8941
Fax +49 2461 61-4823
Web www.grs-sim.de
e-mail: p.carloni@grs-sim.de

EDUCATION

1982: Diploma ('Maturita" Scientifica) with 60/60.

1990: Graduation ('Laurea') in Chemistry at the University of Florence (Italy) with 110/110. Supervisors: Ivano Bertini, Pier Luigi Orioli.

1994: Ph.D. in Chemistry (majoring biophysics), from the University of Florence. Title of the Thesis: 'Theoretical Studies on Metalloproteins'. Supervisors: Lucia Banci, Pier Luigi Orioli (University of Florence), Michele Parrinello (IBM Zurich Research Laboratory).

1990-1991: Visiting scientist at the IBM Research Laboratory, Kingston, NY, USA, with Prof. E. Clementi.

1992: Visiting scientist at the IBM Zurich Research Laboratory, Department of Computational Physics, Ruschlikon, Switzerland, with Dr. Michele Parrinello.

PROFESSIONAL EXPERIENCE

1993-94: Postdoc at the Department of Chemistry, University of Florence and visiting scientist at the Zurich IBM Research in the Lab. of M. Parrinello (Ruschlikon, Switzerland).

1994: Assistant professor in Chemistry at the University of Florence (Italy).

1995-1997: On leave at the University of Florence and Researcher at the IBM, Zurich Research Lab.

1998-2000: Assistant professor in Chemistry at SISSA, Trieste, Italy.

1998-2008: Responsible for the Biophysics Line of Research of the Psi-k European Electronic Structure Network (www.psi-k.org).

2000: Associate professor in Chemistry at SISSA.

2003-2008: Head of the Research Line in Biophysics of the Democritos DEMOCRITOS (National Simulation Center of the Italian *Istituto Nazionale per la Fisica della Materia,* INFM)) in Trieste. Head of the Statistical and Biological Physics Sector.

2004-2009: Full professor in Chemistry at SISSA.

2006-2009 Responsible for SISSA of the Project on Neurosciences and Robotics of the Italian Institute of Technology (www.iit.it).

2009- Full professor (W3) in Theoretical and Computational Biophysics at the German Research School (GRS) of Juelich Research Center (Forschungszentrum Jülich) and of the RWTH-University of Aachen.

2012- Director of the Institute for Computational Biomedicine (IAS-5), Institute for Advanced Simulation, Forschungszentrum Jülich.

RESEARCH INTERESTS

Molecular simulation and bioinformatics approaches to the investigation of problems in the area of biophysical chemistry and molecular medicine. Most of the work is in collaboration with experimental groups.
h-index = 35

SOCIETY MEMBERSHIPS

American Chemical Society
Biophysical Society
German Biophysical Society
PRACE Scientific Steering Committee
JARA-HPC (Jülich Aachen Research Alliance)
Member of the Faculty of Structural and Genomics at SISSA (Trieste, Italy)

REFEREE FOR:

Science, PNAS, Nature Chem. Biol., J. Am. Chem. Soc., J. Phys. Chem., Phys. Rev. Lett., FEBS Lett., Biochemistry, Biophys. J.

EDITORIAL EXPERIENCE:

Editorial Manager *for the Journal: Proteins: Structure, Function, Bioinformatics*
Editor *for the Journal PlosONE.*

FUNDED GRANTS

1998: Quantum description of H-bonding in biological systems: **€ 100,000**. Grant from the Italian Region Friuli Venezia Giulia.

2001: Structural inorganic biology in the post-genomic era: methodologies and "targeting": **€ 28,000**: Grant of the Italian University Minister and SISSA.

2002: 'Molecular modeling of anti-Alzheimer's targets' **€ 40,440**. Grant from the Biotechnological company Lay-Line Genomics, Rome (Italy).

2003: Role of Zn in enzymatic systems and in protein-protein interactions investigated by molecular dynamics simulations: **€ 31.300**. Grant of the Italian University Minister and SISSA.

2003: 'Structural inorganic biology in the post-genomic era: methodologies and targeting': **€ 28,000**: Grant of the Italian University Minister and SISSA.

2003: "Computer Modeling of the Wild-type and Mutated HCN Ion Channels: Structure and Function": **€ 32,300**. Grant from Glaxo-Wellcome, Stevenange, UK.

2004: "Interaction between HIV-1 Tat and its molecular targets: Molecular modeling and in vivo experiments" **€ 44,400**. Grant from the Regione Friuli Venezia Giulia.

2004: 'A new approach to drug design': **€ 30,000** from the Grant of the Italian University Minister.

2004: Two grants for PhD students **(€ 60,000)** given by the Italian Minister of Education for "" Theoretical Investigation of Drug/Target interactions"".

2005 'Theoretical Investigation of proteins involved in Alzheimer's Disease', **€ 200,000** Grant of the Italian University Minister.

2005: Grant for mobility between Italy and Argentina: 'Theoretical Investigations on Metallo Beta-Lactamases' **€ 10,000**.

2005: GRAND grant for "Molecular simulation of neurodegenerative diseases" **(€ 60,000)**.

2006: Telethon Grant for investigation of Parkinsons" Disease: **€ 60,000**.

2006-2008: Grant from the "Instituto Italiano di Tecnologia(IIT)" **(€ 120,000)** for investigation of neurodegenerative disease and of the molecular mechanism of the olfaction.

2006: Grant FVG for "Action of Anticancer agents"**(€ 10,000)**.

2006: Grant FVG for "Action of beta-lactamases" **(€ 10,000)**.

2007: Grant from Illy-Coffee ' Molecular basis of Olfaction and Taste' **(€ 30,000)**.

2009: COFIN from Italian Murst, on neurodegeration **(€ 30,000)**.

2010 NanoCancer Grant from FVG **(€ 40,000)**.

2010-2013: DFG Grant for "Computerstudien zur Physik von Ionen Kanälen" / "Ion Permeation in the Single Channel of the Bacterials Porin NanC: an integrated *in silico* and *in vitro* approach" **(€ 326,000)**.

2011: BANDO AIDS Grant for "Targeting HIV transcription to control infection and to purge post-integrative latency" **(€ 30,000)**.

2011: Nano Cancer Grant for "Investigating proteins involved in human tumor" **(€ 30,000).**

2011-2012: DFG International Cooperation Grant for the "Molecular basis of odorant ligands recognition: a computational study" project in collaboration with Prof. Hoang Zung, Director of the Institute for Science an Technology, Vietnam National University, Ho Chi Minh City (Vietnam) **(€ 19,000).**

2011-2013: PT-DLR International Office BMBF grant for the "International Co-operation Germany / Argentina: Hybrid Coarse grained – atomistic molecular dynamics applied to the study of cold-adaption in hemproteins from Antartic fishes" project in cooperation with Prof. Dario Estrin's group of the University of Buenos Aires (Argentina) **(€ 8,400).**

2012-2015: DFG Grant for "Prediction of structural properties of cisplatin/protein adducts from QM/MM methods" **(€ 159,500).**

In addition, I have contributed to grants with other researchers:

2002: *Ab initio* approach to rational design of drugs targeting proteins involved in neurodegenerative diseases. Computational physics colleagues in SISSA: **€ 1,000,000**. Grant of the Italian University Minister and SISSA. Headed by Prof. Stefano Baroni (Condensed Matter Theory Sector, SISSA).

2002: "Structural and molecular mechanisms of cyclic nucleotide gated channels: **$ 350,000.** HFSP Grant, headed by Prof. V. Torre (SISSA).

RECENTLY FUNDED GRANTS FOR COMPUTING (2010-2012)

2010: First call for the PRACE supercomputing infrastructure: fully granted 48,117,842 core-hours on the JUGENE supercomputer at the Jülich Supercomputing Center for the project '*Ab initio* molecular dynamics simulations of proton transport in a biological ion channel'.

2010: Fully granted access of 288,000 core-hours on the JUROPA supercomputer at the Jülich Supercomputing Center for the NIC project 'Optical properties of fluorescent probes in a protein matrix.'

2010: Fully granted access of 384,000 core-hours on the JUROPA supercomputer at the Jülich Supercomputing Center for the NIC project 'Structural predictions of cisplatin/transplatin-Mets7 adducts from hybrid CPMD/MM calculations.'

2010: Fully granted access of 192,000 core-hours on the JUROPA supercomputer at the Jülich Supercomputing Center for the NIC project 'Water ligand exchange of the Zn^{2+} ion in aqueous solution: A first principle metadynamics study.'

2010: Early Access call for PRACE supercomputing infrastructure: Proposal 'Excess proton at water/hydrophilic interface' for 40,468,480 core-hours on the JUGENE machine. It ranked 3 out of 69 received proposals and it was fully granted.

2011: Fully granted access of 336,000 core-hours on the JUROPA supercomputer at the Jülich Supercomputing Center for the NIC project 'Ion permeation through the Bacterial Porin'.

2011: Fully granted access of 144,000 core-hours on the JUROPA supercomputer at the Jülich Supercomputing Center for the NIC project 'Study of cisplatin binding to Atox1 and ATP7B proteins from QM/MM and replica exchange simulations.'

2011: Fully granted access of 336,000 core-hours on the JUROPA supercomputer at the Jülich Supercomputing Center for the NIC project 'A replica exchange with solute tempering study of the partially unfolded G-protein UreG.'

2011: Fully granted access of 2477260.8 core-hours on the JUGENE supercomputer at the Jülich Supercomputing Center for the NIC project 'Role of conformational selection for the nerve growth factor interactions with its receptors,'

2011: Fully granted access of 192,000 core-hours on the JUROPA supercomputer at the Jülich Supercomputing Center for the NIC project 'Absorption Spectroscopy of Protein-Based Fluorescent Bio-sensors.'

2011: PRACE Preparatory Access call: granted 50,000 core-hours for the CURIE machine at the GENCI/CEA on TGCC in Bruyeres-le-Chatel (France) for the project 'Ion permeation in the single of the bacterial porin NanC'.

2012: Fully granted access of 259,200 core-hours on the JARA-HPC partition of the RWTH compute cluster at the Aachen Rechenzentrum for the project 'Regulation Mechanism of SIRT2 - A Promising Pharmaceutical Target Protein for Age-related Diseases.'

2012: Fully granted access of 777,000 core-hours on the JARA-HPC partition of the RWTH compute cluster at the Aachen Rechenzentrum for the project 'Conformational heterogeneity of flexible proteins probed through metadynamics simulations.'

2012: Fully granted access of 40,000 core-hours on the JARA-HPC partition of the RWTH compute cluster at the Aachen Rechenzentrum for the project 'From the chimeric human/mouse prion proteins to the molecular basis of prion diseases.'

2012: Fully granted access of 82,800 core-hours on the JARA-HPC partition of the RWTH compute cluster at the Aachen Rechenzentrum for the project 'Ligand screening in G-protein coupled receptors:insights from bioinformatics and MM/CG simulations.'

ORGANIZATIONAL EXPERIENCE

1. ICTP workshop on Structure and Function of Biomolecules, Trieste 1998.

2. INFM National Meeting on Computational Methods in Biological Systems, Catania, Italy 1999.

3. CECAM - PsiK workshop on Ab-initio modelling in the biological sciences, Lyon, France, 2001.

4. ICTP Conference on Interaction and Assembly of Biomolecules, Trieste 2001.

5. ICTP College on Biophysics: From Molecular Genetics to Structural Biology', Trieste 2001.

6. CECAM workshop on 'Ion Channels: from Biology to Physics', Lyon, France 2002.

7. ICTP-INFM Conference on 'New Frontiers in Nano-Biotechnology: Monitoring Protein Function with Single-Protein Resolution', Trieste, 2003.

8. Psi-k Workshop on '*Ab Initio* Modelling in Biological Systems', May 2004, Trieste.

9. 'Biophysics Symposium' of the Psi-k conference, Schwäbisch Gmünd, Germany, September 2005.

10. ICTP Conference on "Drug development for the third world", Trieste, June 2006.

11. Psi-k workshop on *ab initio* modelling of biomolecules: methods and applications, Leiden, July 2006.

12. CECAM workshop in Hybrid Atomistic Methods for Materials and Biological Systems, Lyon, July 2006.

13. CECAM workshop on DNA: From Quantum to Coarse Grain, Lyon, France, October 2006.

14. CPMD2008 ICTP conference on modeling and computation of structure and dynamics of condensed phase systems, Trieste, June 2008.

15. Ab Initio Modelling in Applied Biosciences: Structure, Dynamics and Function, Uppsala University, December 2008.

16. International Workshop on Computational Biophysics (IWCBP-1), Ho Chi Minh City, Vietnam, February 2010.

17. Workshop on Computational Modelling and Simulation of Biological Systems, Unidad de Gestión Cientifica, Institut Pasteur Montevideo, Uruguay, February-March 2010.

18. Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics (CECAM Conference), SISSA, Trieste, Italy, July 2010.

19. Conference on Molecular Aspects of Cell Biology: A Perspective from Computational Physics, ICTP Miramare, Trieste, Italy, October 2010.

20. Workshop on Large-Scale Computer Simulation, German Research School Jülich / Aachen, Germany, March 2011.

21 CPMD 2011 "Extending the limits of Ab initio Molecular Dynamics Simulations for Chemistry, Materials Science and Biophysics", Barcelona, Spain, September 2011

22. CECAM Workshop at EPFL, Lausanne, Switzerland: Molecular Simulations of Membrane Proteins: From Biophysics to Pharmacological, March 2012

23. Workshop - Oak Ridge National Laboratory (Joint Institute for Computational Sciences (JICS) German Research School (GRS) Joint Workshop on Large Scale Computer Simulation), Knoxville, Tennesse, USA, April 2012.

INVITED LECTURES

In Conferences/Workshops

1992

1. Workshop on Advanced Calculations in Chemistry, Montelivretti, Italy.

1993

2. SISSA Discussion Day, SISSA, Trieste, Italy.

1994

3. September: European Bioinorganic Conference (EUROBIC II), Florence, Italy.

1995

4. June: ICTP International School of Computational Material Science, Trieste, Italy.
5. September: Italian National Congress of Crystallography, Taormina, Italy.

1996

6. August: European Bioinorganic Conference EUROBIC III, Noordwijkerhout, The Netherlands.

1997

7. March: NATO Advanced Workshop - Molecular Modeling and Dynamics of Biological Molecules Containing Metal Ions, S. Miniato, Italy.

1998

8. May: CECAM Workshop on Combined Quantum Mechanical -Classical Hybrid Methods for the Simulation of Chemical Reactions, Lyon, France.
9. June: CECAM Workshop on Computational Exploration of Energy Landscapes in Protein Dynamics, Turin, Italy.
10. August: European Bioinorganic Conference (EUROBIC IV), Sevilla, Spain.

1999

11. January: Car-Parrinello Molecular Dynamics Conference, Schloss Ringberg, Munich, Germany.
12. March: XVIII Congress of Theoretical Physics, Fai Della Paganella, Italy.
13. July: CECAM workshop on Molecular Dynamics Simulations of Lipid Membranes and Membrane Associated Proteins, Lyon.
14 August: ICTP Workshop on Calculation of Material Properties Using Total Energy and Force Methods and ab initio Molecular Dynamics, Trieste, Italy.
15. September: Fifth European SGI/Cray MPP Workshop, Bologna, Italy.

2000

16. March: International Conference on Research Trends in Science and Technology, Beirut, Lebanon.
17. March: 15 Years of Car-Parrinello in Physics and Chemistry, Minneapolis, USA.
18. August: Psi-k 2000 Conference, Schwabisch Gmund, Germany.
19. August: Statistical Mechanics of Complex Systems Conference, Bled, Slovenia.
20. October: CECAM workshop on Molecular modeling methods for the development of NMR in structural biology, Lyon, France.
2001

21. January Car-Parrinello Molecular Dynamics Meeting, Schloss Ringberg, Germany.
22. March: 2001 International Conference on Computational Nanoscience, Helton Head Island, SC, USA.
23. April: American Chemical Society Meeting, S. Diego, CA, USA.
24. June: CECAM workshop on New methods for combining Born-Oppenheimer ab initio calculations and empirical force fields in large scale simulation studies, Lyon, France.
25. June: Thirteenth Annual Workshop on Recent Developments in Electronic Structure Algorithms, Princeton, NJ, USA.
26. June: International Workshop on Protein Folding, Structure and Design, ICTP Workshop, Trieste, Italy.
27. September: 9th Swiss Workshop of Methodology in Receptor Research, Zurich, Switzerland.
28. October: ICGEB meeting on The Biology of the Post-Genomic Era, Trieste, Italy.
29. November: Workshop on Modeling Quantum Chemistry, Molecular dynamics and Spectroscopy of Blue Copper proteins and Their Protein Matrices, Leiden, The Netherlands.

2002

30. January: School on Biophysics: Water in Biomolecules, Venice, Italy.
31. March: US-Italy Workshop on Frontiers in Materials Research, Nanoscience and Nanotechnology Washington, DC, USA.
32. June: Italian Chemical Society Meeting, Verona, Italy.
33. July: Quantum Bioinorganic Chemistry Conference, Lund, Sweden.
34. August: WATOC Conference, Lugano, Switzerland.
35. September: EURESCO Conference on Computational Biophysics: Integrating Theoretical Physics and Biology, San Feliu, Spain.
36. December: COFIN meeting: Inorganic structural biology in the post-genomic era: methodologies and targeting, Florence, Italy

2003

37. January: ICTP XI International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, Trieste, Italy.
38. July: Second Joint French - Swiss Meeting on Medicinal Chemistry, Beaune, France.
39. September: Biocrystallography course: from gene to drug, Trieste, Italy.
40. September: Workshop on Ab initio Electrons Excitations Theory: Towards Systems of Biological Interest, San Sebastian, Spain.
41. November: Argentine Chemical Society: Meeting of the Organic Chemistry Section, Rosario, Argentina.
42. December: Italian Chemical Society: Meeting on the Computational Chemistry Division, Siena, Italy.

2004

43. March: EURESCO Conference on molecules of biological interest in the gas phase, Exeter, UK.
44. June: Workshop on Mathematical Virology, Oxford, UK.
45. June: Workshop on Soft Matter Physics, Dubrovnik, Croatia.
46. July: EMBO School of Biophysics, Verona, Italy.

2005

47. March International Conference on Research Trends in Science and Technology, Beirut, Lebanon.
48. March ACS National Meeting, San Diego, CA, USA.
49. April Workshop on Biophysics, Oxford, UK.
50. May: Workshop on Beta-Lacamases, Leonessa, Italy.
51. June: Workshop on Drug Design, Siena, Italy.
52 July: ERICE School CSCM 2005, Erice, Italy.
53. August: Telluride Workshop on Protein Dynamics, Telluride, CO, USA.
54. August: ACS National Meeting, Washington, USA.
55. August: Nancy EUROCHEM conference, Nancy, France.
56. September: Biomolecular Simulations 2005 Meeting, Bordeaux, France.
57. September: CPMD Meeting, Ascona, Switzerland.
58. November: Biological Dynamics: from Molecules to Cell, Amsterdam, The Netherlands.
59. December: Pacifichem, Honolulu, Hawai, USA.

2006

60. March: CINECA Meeting, Bologna, Italy.
61. June: ICTP Conference on Drug development for the third world, Trieste, Italy.
62. June: Trieste Conference on van der Waals Interactions, Trieste, Italy.
63. July: Varenna School on Protein Folding and Design, Varenna, Italy.
64. August CCP 2006: Conference on Computational Physics, Gyeongju, Korea.
65. October: CECAM workshop on Recent Advance in Modeling DNA, Lyon, France.
66. November: Argentinean National Biophysics Conference, Rosario, Argentina.
67. November: NMR Meeting of the Argentinean Biophysics Society, Rosario, Argentina.

68. November: EURESCO CONFERENCE on Inorganic Chemistry: Metal-Nucleic Acid interactions, Athens, Greece.

2007

69. January: 'Winter School on Physical Organic Chemistry', Bressanone, Italy.
69. April: Ab initio modeling of Biomolecules: Towards Computational Spectroscopy, Rome, Italy.
70. May: International Drug Discovery Science and Technology (IDDST)Conference, Shangai, China.
71. August: Conference on Mathematical Virology, Edimburgh, UK.
72. September: CCP 2007: Conference on Computational Physics, Bruxelles, Belgium.
73. September: CECAM workshop Ionic Transport: from Nanopores to Biological Channels, Lyon, France.
74. September: International Conference of Computational Methods in Sciences and Engineering, Corfu, Greece.
75. September: 2nd Opatija Meeting On Computational Solutions in the Life Sciences,Opatija, Croatia.
78. November: 5th Anniversary Congress of International Drug Discovery Science and Technology, Xi'an, China.

2008

79. April: MGMS Spring Meeting: Bio-inorganic Chemistry, Cardiff, UK.
80. June: Drug Design and Discovery for Developing Countries, Trieste, Italy.
81. June: Pushing the Boundaries of Biomolecular Simulations", Ascona, Switzerland
82. July: 1st World Summit on Antivirals, Kunming, China.
83. September: 6th Congress on Electronic Structure: Principles and Applications - ESPA 2008, Palma de Mallorca, Spain.
84. October: 6th International Drug Discovery, Science and Technology (IDDST 2008), Beijing, China.
85. December: Ab Initio Modelling in Applied Biosciences: Structure, Dynamics and Function, Uppsala, Sweden.
86. December: 'Winter Modeling 2008, Pisa, Italy.

2009

87. January: 'Biomolecular Simulation Meeting 2009', York, UK.
88. June: '2nd Conference on Drug Development for the Third World: from Computational Molecular Biology to Experimental Approaches', Trieste, Italy.
89. July: ' Conference on Antivirals', Beijing, China.
90. August: 'SEADIM Conference', Habana and Varadero, Cuba.

2010:

91. February-March: Workshop on Computational Modelling and Simulation of Biological Systems, Unidad de Gestión Cientifica, Institut Pasteur Montevideo, Uruguay.
92. April: TYC Workshop on Biological Interfaces, King's College London, England.
93. June: Multiscale modeling for engineering applications: from atoms to macroscopic systems, University of Turin, Italy.
94. July: Role of first principle calculations for mechanistics systems biology, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany.
95. August: 3rd Mathematical Virology Workshop Ambleside, The University of York, Cumbria, England.
96. September: PSI_K Conference 2010, Henry Ford Building, Berlin, Germany.97. September: Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Leipzig, Germany.
98. October: BIT's 8th Annual Congress of 2010 International Drug Discocery Science and Technology, Beijing, China.
99. October: BIT's 1st Annual World Congress of NanoMedicine-2010, Beijing, China.

100. November, EESI Workshop, Amsterdam, Netherlands.
101. November: BioScience 2010 - Workshop on expanding the frontiers of biomolecular science, Forschungszentrum Jülich, Germany.
102. December: Lincei Meeting 2010 – Accademia Nazionale Dei Lincei, Rome, Italy.
103. December: HPC-Anwenderforum, Dresden, Germany.
104. December: Exascale Meeting, Barcelona, Spain.

2011:

105. March: Workshop on Large-Scale Computer Simulation, German Research School for Simulation Sciences, Aachen / Jülich, Germany.
106. March: IPAM Long Program- Navigating Chemical Compound Space for Materials and Bio Design (CCS2011), Los Angeles, USA.
107. April - Fet 11 – The European Future Technologies Conference and Exhibition, Budapest, Hungary.
108. May - Mainz Materials Simulation Days 2011, Mainz, Germany.
109. June: Inaugurazione BIOMETION Padova, Italy.
110. June: TheoBio2011 – 5th Theoretical Biophysics International Symposium, Madeira, Portugal.
111. July: Scuola Nazionale Di Chimica Bioinorganica, University of Siena, Italy.
112. July: Workshop on Structural Bioinformatics and Computational Biophysics, SISSA – University of Trieste, Italy.
113. July: SEADIM – 8th Seminars of Advanced Studies on Molecular Design and Bioinformatics, University of Havana, Cuba.
114. July: CBSC Workshop: From Computational Biophysics to Systems Biology 2011, FZ / JSC Jülich, Germany.
115. September: CECAM Workshop: Combining experimental and computational techniques to study protein behaviour, Lugano, Switzerland.
116. October: CECAM Conference: Innovative Approaches to Computational Drug Discovery. Lausanne, Switzerland.
117. October: 1st CAS-HGF Workshop on Supercomputing Beijing, China.
118. October: FET-HBP Pharma Application Workshop at EPFL, Lausanne, Switzerland.
119. December: FET-HBP Pharma Application Workshop at EPFL, Lausanne, Switzerland.
2012:

120. January: Fourth International Conference on the Development of Biomedical Engineering (BME4), Ho Chi Minh City, Vietnam.
121. March: Jülich Winter School 2012, Forschungszentrum Jülich, Germany.
122. May: Leermakers Symposium, Wesleyan University Middletown, CT.
123. May: CECAM 2012 Workshop on Alzheimer's disease, Paris, France.
124. May/June: Intel Leadership Conference on HPC for Life Science, Brussels, Belgium.
125. June: CECAM Workshop "DNA sequencing and detection with nanoprobes", Pisa, Italy.
126. July: X Girona Seminar on Theoretical and Computational Chemistry for the Modeling of Biochemical Systems: From Theory to Applications, Girona, Spain.
127. September: Workshop FZ Jülich / AlQuds University 2012, Forschungszentrum Jülich, Germany.
128. October: MMM 2012 - Multiscale Materials Modeling Conference, Singapore.

In Universities and Research Institutes

1995

1. August: Pharmacy Department, ETH, Zurich, Switzerland.

1996

2. September: The Beckman Institute of the University of Illinois, Urbana-Champaign, IL, USA

3. November: C4 Workshop -Use of Fast Computers in Molecular Chemistry - ETH, Zurich, Switzerland.

1997

4. February: Chemistry Department, Dortmund University, Germany.
5. October: Biophysics Department, ETH, Zurich.

1998

6. January: Joint ICTP/SISSA Condensed Matter Seminar, Trieste, Italy.
7. July: Institute of Structural Biology Jean-Pierre Ebel', Grenoble, France.
8. October: National Institute of Chemistry, Lubljiana, Slovenia.
9. October: Department of Chemistry, University of Zagreb, Croatia.

1999

10. January: Chemistry Department, Trieste University, Trieste. Italy.
11. July: The Beckman Institute of the University of Illinois, Urbana-Champaign, IL, USA.
12. July: Department of Theoretical Biophysics, Los Alamos National Labs, Los Alamos (NM), USA.
13. July: Chemistry Department, University of Princeton, Princeton (NJ), USA.
14. September: Biophysics Department, University of Rosario, Argentina.
15. September: Chemistry Department, University of Buenos Aires; Argentina.
16. December: Chemistry Department, University of Siena, Italy.

2000

17. March: Physics Department, UCSD, San Diego, CA, USA.
18. March: Chemistry Department, UC Irvine, CA, USA.
19. March: The Beckman Institute of the University of Illinois, Urbana-Champaign, IL (USA).
20. April: Physics Department, University of Padua, Italy.
21. June: National Institute of Chemistry, Ljubljana, Slovenia.
22. July: Fritz-Haber Institute, Berlin, Germany.
22. September: Pharmacy Department, University of Madison, WC, USA.
23. October: Department of Biology, University of Osnabrueck, Germany.
24. December: Department of Physics, University of Florence, Italy.

2001

25. March: Department of Biophysics, Wesleyan University, Middletown, CT, USA.
26. March: Chemistry Department, Univ. of Pennsylvania, Philadelphia, USA.
27. July: Department of Physics, University of Modena, Italy.
28. October: Chemistry Department, University of Lund, Sweden.

2002

29. March: Glaxo Research Center, Verona, Italy.
30. September: Department of Pharmacy, Genome Bioinformatics Research Laboratory, University Pompeu Fabra, Barcelona, Spain.

2003
31. March: Venetian Institute of Molecular Medicine, Padua, Italy.
32. May: Department of Physics, University of Modena.
33. June: C4 Workshop -Use of Fast Computers in Molecular Chemistry - ETH, Zurich, Switzerland.
34. November: Department of Biophysics, University of Rosario, Argentina.

2004

35. March: Department of Physics, University of Modena, Italy.
36. March: Department of Chemistry, University of Palermo, Department of Chemistry
37. April: Italian Research Council, Pisa, Italy.

2005

38. March: Department of Chemistry, University of Cambridge, UK.
39. April: Department of Chemistry, University of Lubiana, Slovenia.
40. June: University of Linz, Austria.

2006
41. December: Department of Chemistry, University of Sussex, UK.

2007
42. February: Department of Physics, University of Ho-Chi-Min-City, Vietnam.

2008
42. February: Swinburne University, Melbourne, Australia.
43. September: Scuola Normale Superiore di Pisa, Pisa, Italy.

2009

45. October: University of Bari, Italy
46. November: University of Santa Barbara, CA, USA.

2010

47. December: University of Siena, Siena, Italy.

2011

48. February: Leibniz Institute of Molecular Pharmacology (FMP Berlin)
Berlin, Germany
49. May: University Hospital Aachen, Germany.
50. August: University College Dublin, Ireland.
51. September: University of Southampton, England.
52. October: Johannes Kepler University, Linz, Austria.
53. October: Beijing University of Technology, Beijing, China.
54. December: Biophysical Society Argentina, Buenos Aires, Argentina.

2012

55. February: SISSA, University of Trieste, Italy.
56. June: University of Perugia, Italy.
57. September: Institut de Biologie Physico-Chimique (IBPC), Paris, France.
58. October: Jena University Hospital, Germany.
59. November: Institute of Organic Chemistry and Biochemistry AS CR, Prague, Czech Republic.

EXTERNAL EXAMINER EXPERIENCE

External examiner for the PhD thesis of: (i) E. Sigfridsson, Department of Chemistry, Lund University, Sweden (2002); (ii) Davide Provasi, Department of Physics, University of Milano, Italy (2002); (iii) Lars Olsen, Department of Mathematics and Physics, The Royal Veterinary and

Agricultural University, Frederiksberg, Denmark (2003). (iv) J. Raber, Uppsala, Sweden, July 2007.

HIRING COMMITTEE EXPERIENCE

External member for hiring a full professor in theoretical biophysics at the University of Linz (Austria), October 2008.
External member of commission for hiring an associate professor in experimental biophysics at RWTH, University of Aachen (Germany).

VISITING PROFESSOR EXPERIENCE

- Eight lectures on 'Molecular Modeling of Biological Systems', at the Department of Biophysics, University of Rosario, Argentina, September 1999.

- Eight lectures on 'Protein Physics' at the Department of Physics, University of Modena, Italy, March 2004.

- Three lectures on " Principles and Applications of Biomolecular simulation", Department of Physics, Hanoi University, February 2007.

- Eleven Lectures on 'Molecular Biophysics and Molecular Simulation' Department of Physics, National University of Vietnam, Ho-Chi-Min-City, Vietnam, February 2008.

STUDENTS

-Supervised PhD students

Frank Alber (1996-1998); Lorenzo de Santis (1997-1999); Leonardo Guidoni (1998-2000) Stefano Piana (1998-2000); Sergio Pantano (1999-2001); Maria Lore Sulpizi (1999-2001) Giovanni Settanni (1999-2001); Valeria Costa (1999-2002); Marco Punta (1999-2002) Matteo dal Peraro (2000-2004); Katrin Spiegel (2000-2004); Michele Cascella (2000-2004) Alejandro Giorgetti (2000-2004); Pietro Vidossich (2001-2006); Marco Berrera (2002-2006) Marilisa Neri (2003-2007); Giacomo Fiorin (2003-2006); Vincenzo Carnevale (2003-2007); Kamil Khafizof (2003-2008); Fernando Herrera (2004-2008); Attilio Vargiu (2003-2008); Agata Kranic (2004-2008); Fabio Simona (2004-2008); Vanessa Leone (2005-2009); Rolando Hong (2005-2009);Roberto Marchese (2006-2010); Giulia Rossetti (2006 – 2010); Salvatore Bongarzone (2006-2010), Gianpaolo Chiriano (2006-2010); Valeria Losasso (2006 -2011);

- Current supervising the PhD students:

Xiaojing Cong (2007 -); Trang Do (2009 -); Chuong Nguyen (2009 -); Chao Zhang (2009 -); Qui Vo Cam (2009 -); Domenica Dibenedetto (2010 -); Trung Hai Nguyen (2009 -); Jinyu Li (2011 -).

- Supervised the undergraduate students:

Frank Alber (1996); Matteo dal Peraro (2000);Pietro Vidossich (2002); Paola Lupieri (2006); Michela Candotti (2007).

- Currently Supervising the undergaduate student: Oliver Rusche (2012-)

CURRENT TEACHING ACTIVITY

Courses currently thought at the 2-year GRS Master in Simulation Sciences at the German Research School, Juelich Research Center and RWTH-Aachen:

1. From Molecular to Continuum Physics I (70 hours, Mandatory Course)

2. Simulation Sciences Lab (30 hours, Mandatory Course)

3. Data Analysis and Visualizations (9 hours, Mandatory Course)

4. Computational Molecular Biology (42 hours)

Course taught in the PhD Course in Structural and Functional Genomics in SISSA, Trieste, Italy

1. Biomolecular modeling (15 hours, Mandatory course).