Curriculum Vitæ Alessandro Laio

Professional address

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Education

• February 1995: Degree in Nuclear Engineering ("Laurea") at Politectnico di Torino. Final grade: 110/110 cum laude. Thesis: *A quantum interpretation of the anomalous redshifts in astrophysics and cosmology.* Supervisors: Guido Rizzi and Luigi Accardi (University of Rome II).

• October 1996: Master in Physics at SISSA, Trieste. Thesis: *Interacting hard-core bosons and surface physics.* Supervisor: Giuseppe Santoro.

• Ph.D. degree obtained in October 1999. Thesis: *Simulation of iron at earth's core conditions* . Supervisors: Sandro Scandolo, Guido Chiarotti and Erio Tosatti.

Professional Experience

• February 1995 -September 1995: research work in collaboration with Prof. G. Rizzi and Prof. A. Tartaglia at Politecnico di Torino.

• November 1995- December 1999: graduate studentship at ISAS-SISSA.

• January 2000- December 2001: postdoctoral research assistant in the group of Prof. Ursula Rothlisberger at ETH Zurich.

• January 2002- December 2003: postdoctoral research assistant in the group of Prof. Michele Parrinello in Lugano.

• January 2004-December 2005: Oberassistant in the group of Prof. Michele Parrinello in Lugano.

• January 2006-March 2010: Researcher at SISSA with a *Rientro dei cervelli* scholarship.

• April 2009-November 2012: Director of the SISSA-DEMOCRITOS CECAM Node

• March 2010: Associate Professor at SISSA, Trieste.

• October 2014: Full Professor at SISSA, Trieste

Research grants

- 15 February 2006: 140,000 Euro from the found "Mobilita' di docenti italiani e stranieri impegnati all'estero D.M. 01-02-2005" as PI. Title of the project: *Simulation of Rare Events in Biological Systems*

- 10 November 2011: 290,000 Euro from the found "FIRB-accordi di programma" as local coordinator (PI: Prof. Maurizio Prato), Title of the project: *Approcci nanotecnologici per la teragnostica dei tumori*

- 1 January 2012: 550,000 Euro from the found "AIRC 5 per mille" as local coordinator (PI: Dr. Giuseppe Toffoli), Title of the project: *Application of Advanced Nanotechnology in the Development of Innovative Cancer Diagnostics Tools.*

- June 2012-June 2013 110,000 Euro from the found "FOODCAST" sponsored by Regione Lombardia.

- 2013-2015 55,000 Euro from the foun "PRIN" as local coordinator (PI: Prof. Amos Maritan). Title of the project: *Statistical Physics of Active Matter: Disentangling Complexity Patterns in Biological Systems*

Supervising

I am currently supervising three PhD students:

Year of course	***Name***
II	Elena Facco
IV	Edoardo Sarti
III	Francesca Rizzato

Nine students have already obtained their PhD in SISSA under my supervision:

Year of completion	***Name***	***Present position and Institution***
2014	Ina Bisha	Postdoctoral fellow, University of Munich
2013	Daniele Granata	Postdoctoral fellow, Temple Univ, Philadelphia
2013, co-supervision with Prof. Stefano Baroni	Gianpaolo Gobbo	Research assistant, Univ. Of Edinburgh
2013	Luca Ianiselli	Postdoctoral fellow, ELETTRA, Trieste
2012	Fahimeh Baghal	Postdoctoral fellow,MIT, Boston
2012	Zhaleh Ghemi	Postdoctoral fellow,Univ. Of Illinois, Urbana
2011	Pilar Cossio	Research assistant, MPI Frankfurt
2010, co-supervision with Prof. Erio Tosatti	Yanier Crespo	Postdoctoral fellow, ICTP Trieste
2009	Fabrizio Marinelli	Research assistant, NIH, Washington, USA

My research group also includes five postdoctoral fellows:

Position	*Name*	*Funded by*
Ricercatore TD	Alex Rodriguez	FIRB Grant
Ricercatore TD	Ivan Gladich	FIRB Grant
Assegnista di ricerca	Anna Battisti	AIRC Grant
Assegnista di ricerca	Michele Allegra	SISSA
Assegnista di ricerca	Maria D'Errico	PRIN Grant

Finally, four postdoctoral fellows left my group, and are currently employed in other institutions:

Name	*Period of stay at SISSA*	*Present position and Institution*
Rolando Hong	2012-2013	Postdoctoral fellow, IIT Genova
Xevi Biarnes	2009-2011	Assistant Professor, Universitat Ramon Liull, Barcelona
Xiaoliang Hu	2011-2013	Postdoctoral fellow, EPFL Lausanne
Fabio Pietrucci	2007-2009	Senior research assistant, EPFL, Lausanne

Publications and scientific impact

Number of publications: 87

Times cited (ISI): 5558

Times cited in 2014 (ISI): 796

H-index (ISI): 37

1. Bisha I, Rodriguez A., Laio A., Magistrato A., *Metadynamics Simulations Reveal a Na+ Independent Exiting Path of Galactose for the Inward-Facing Conformation of vSGLT,* **PLOS Comp. Biol.**, 2015, 10, e1004017

2. Rodriguez A., Laio A, *Clustering by fast search-and-find of density peaks,* **Science**, 2014, 344, 6191

3. Prestipino S., Laio A., Tosatti E. *Shape and area fluctuation effects on nucleation theory,* **J. Chem. Phys.**, 2014, 140, 094501

4. Sarti E., Zamuner S., Cossio P., Laio A., Seno F., Trovato A. *BACHSCORE. A tool for evaluating efficiently and reliably the quality of large sets of protein structures,* 2013, **Comp. Phys. Comm.**, 184, 2860

5. Granata, D., Camilloni, C., Vendruscolo, M., Laio, A., *Characterization of the free-energy landscapes of proteins by NMR-guided metadynamics,* 2013 **Proceedings of**

the National Academy of Sciences of the United States of America, 110, 6817

6. Baftizadeh, F., Pietrucci, F., Biarnés, X., Laio, A., *Nucleation process of a fibril precursor in the C-terminal segment of amyloid-β*, 2013 **Phys. Ref. Lett.** 110, 168103

7. Prestipino, S., Laio, A., Tosatti, E., *A fingerprint of surface-tension anisotropy in the free-energy cost of nucleation*, 2013 **J. Chem. Phys. , 138, 064508**

8. Bisha, I., Laio, A., Magistrato, A., Giorgetti, A., Sgrignani, J., , A candidate ion-retaining state in the inward-facing conformation of sodium/galactose symporter: Clues from atomistic simulations, 2013, ***J.Chem. Th. And Comp.,*** *9, 1240*

9. Hu, X.L., Piccinin, S., Laio, A., Fabris, S, *Atomistic structure of cobalt-phosphate nanoparticles for catalytic water oxidation. 2012* ***ACS Nano*** *6, 10497*

10. Gobbo, G., Laio, A., Maleki, A., Baroni, S. *Absolute transition rates for rare events from dynamical decoupling of reaction variables 2012* ***Physical Review Letters*** *109, 150601*

11. Ghaemi, Z., Minozzi, M., Carloni, P., Laio, A. *A novel approach to the investigation of passive molecular permeation through lipid bilayers from atomistic simulations* 2012 **Journal of Physical Chemistry B** 116, 8714

12. Prestipino, S., Laio, A., Tosatti, E. *Systematic improvement of classical nucleation theory* 2012 **Physical Review Letters** 108, 225701

13. Cossio, P., Granata, D., Laio, A., Seno, F., Trovato, A. *A simple and efficient statistical potential for scoring ensembles of protein structures* 2012 **Scientific Reports** 2, 351

14. Hong R.P., Pavan, S., Benedetti, F., Tossi, A., Savoini, A., Berti, F., Laio, A. *Designing short peptides with high affinity for organic molecules: A combined docking, molecular dynamics, and Monte Carlo approach* 2012 **Journal of Chemical Theory and Computation** 8, 1121

15. Baftizadeh, F., Biarnes, X., Pietrucci, F., Affinito, F., Laio, A. *Multidimensional view of amyloid fibril nucleation in atomistic detail* 2012 **Journal of the American Chemical Society** 134, 3886

16. Biarnes, X., Pietrucci, F., Marinelli, F., Laio, A. *METAGUI. A VMD interface for analyzing metadynamics and molecular dynamics simulations* 2012 **Computer Physics Communications** 183, 203

17. Crespo, Y., Laio, A., Santoro, G.E., Tosatti, E. *Theory of the reentrant quantum rotational phase transition in high-pressure HD* 2011 **Physical Review B** 84 144119

18. Rossetti, G., Cossio, P., Laio, A., Carloni, P. *Conformations of the Huntingtin N-term in aqueous solution from atomistic simulations* 2011 **FEBS Letters** 585 3086

19. Cardamone, L., Laio, A., Torre, V., Shahapure, R., DeSimone, A. *Cytoskeletal actin networks in motile cells are critically self-organized systems synchronized by mechanical interactions* 2011 **Proceedings of the National Academy of Sciences of the United States of America** 108 13978

20. Liu, L.-M., Laio, A., Michaelides, A. *Initial stages of salt crystal dissolution determined with ab initio molecular dynamics* 2011 **Physical Chemistry Chemical Physics** 13 13162

21. Cossio, P., Laio, A., Pietrucci, F. *Which similarity measure is better for analyzing protein structures in a molecular dynamics trajectory?* 2011 **Physical Chemistry Chemical Physics** 13 10421

22. Zhai, Y., Laio, A., Tosatti, E., Gong, X.-G. *Finite temperature properties of clusters by replica exchange metadynamics: The water nonamer* 2011 **Journal of the American Chemical Society** 133 2535

23. Cossio, P., Trovato, A., Pietrucci, F., Seno, F., Maritan, A., Laio, A. *Exploring the universe of protein structures beyond the protein data bank* 2010 **PLoS Computational Biology** 6 e1000957

24. Crespo, Y., Marinelli, F., Pietrucci, F., Laio, A. *Metadynamics convergence law in a multidimensional system* 2010 **Physical Review E** 81 55701

25. Shahapure, R., Difato, F., Laio, A., Bisson, G., Ercolini, E., Amin, L., Ferrari, E., Torre, V. *Force generation in lamellipodia is a probabilistic process with fast growth and retraction events* 2010 **Biophysical Journal** 98 979

26. Cossio, P., Marinelli, F., Laio, A., Pietrucci, F. *Optimizing the performance of bias-exchange metadynamics: Folding a 48-residue LysM domain using a coarse-grained model* 2010 **Journal of Physical Chemistry B** 114 3259

27. Pietrucci, F., Laio, A. *A collective variable for the efficient exploration of protein beta-sheet structures: Application to SH3 and GB1* 2009 **Journal of Chemical Theory and Computation** 5 2197

28. Michel, C., Laio, A., Milet, A. *Tracing the entropy along a reactive pathway: The energy as a generalized reaction coordinate* 2009 **Journal of Chemical Theory and Computation** 5 2193

29. Pietrucci, F., Marinelli, F., Carloni, P., Laio, A. *Substrate binding mechanism of HIV- 1 protease from explicit-solvent atomistic simulations* 2009 **Journal of the American Chemical Society** 131 11811

30. Crespo, Y., Laio, A., Santoro, G.E., Tosatti, E. *Calculating thermodynamics properties of quantum systems by a non-Markovian Monte Carlo procedure* 2009 **Physical Review E** 80 15702

31. Marinelli, F., Pietrucci, F., Laio, A., Piana, S. *A kinetic model of Trp-cage folding from multiple biased molecular dynamics simulations* 2009 **PLoS Computational Biology** 5

e1000452

32. Mones, L., Kulhanek, P., Simon, I., Laio, A., Fuxreiter, M. *The energy gap as a universal reaction coordinate for the simulation of chemical reactions* 2009 **Journal of Physical Chemistry B** 113 7867

33. Laio, A., Gervasio, F.L. *Metadynamics: A method to simulate rare events and reconstruct the free energy in biophysics, chemistry and material science* 2008 **Reports on Progress in Physics** 71 126601

34. Piana, S., Laio, A. *Advillin folding takes place on a hypersurface of small dimensionality* 2008 **Physical Review Letters** 101 208101

35. Pietrucci, F., Bernasconi, M., Laio, A., Parrinello, M. *Vacancy-vacancy interaction and oxygen diffusion in stabilized cubic ZrO2 from first principles* 2008 **Physical Review B** 78 94301

36. Micheletti, C., Bussi, G., Laio, A. *Optimal Langevin modeling of out-of-equilibrium molecular dynamics simulations* 2008 **Journal of Chemical Physics** 129 74105

37. Colombo, M.C., VandeVondele, J., Van Doorslaer, S., Laio, A., Guidoni, L., Rothlisberger, U. *Copper binding sites in the C-terminal domain of mouse prion protein: A hybrid (QM/MM) molecular dynamics study* 2008 **Proteins: Structure, Function and Genetics** 70 1084

38. Piana, S., Laio, A., Marinelli, F., Van Troys, M., Bourry, D., Ampe, C., Martins, J.C. *Predicting the Effect of a Point Mutation on a Protein Fold: The Villin and Advillin Headpieces and Their Pro62Ala Mutants* 2008 **Journal of Molecular Biology** 375 460

39. Biarnes, X., Ardavol, A., Planas, A., Rovira, C., Laio, A., Parrinello, M. *The conformational free energy landscape of glucopyranose. Implications for substrate preactivation in Î_-glucoside hydrolases* **2007 Journal of the American Chemical Society** 129 10686

40. Piana, S., Laio, A. *A bias-exchange approach to protein folding* 2007 **Journal of Physical Chemistry B** 111 4553

41. Bulo, R.E., Donadio, D., Laio, A., Molnar, F., Rieger, J., Parrinello, M. *Site binding of Ca2+ ions to polyacrylates in water: A molecular dynamics study of coiling and aggregation* 2007 **Macromolecules** 40 3437

42. Maurer, P., Laio, A., Hugosson, H.W., Colombo, M.C., Rothlisberger, U. *Automated parametrization of biomolecular force fields from Quantum Mechanics/Molecular Mechanics (QM/MM) simulations through force matching* 2007 **Journal of Chemical Theory and Computation** 3 628

43. Michel, C., Laio, A., Mohamed, F., Krack, M., Parrinello, M., Milet, A. *Free energy ab Initio metadynamics: A new tool for the theoretical study of organometallic reactivity? Example of the C-C and C-H reductive eliminations from platinum(IV) complexes* 2007 **Organometallics** 26 1241

44. Laio, A., Parrinello, M. *Computing free energies and accelerating rare events with metadynamics* 2006 **Lecture Notes in Physics** 703 315

45. Laino, T., Mohamed, F., Laio, A., Parrinello, M. *An efficient linear-scaling electrostatic coupling for treating periodic boundary conditions in QM/MM simulations* 2006 **Journal of Chemical Theory and Computation** 2 1370

46. Roehrig, U.F., Laio, A., Tantalo, N., Parrinello, M., Petronzio, R. *Stability and structure of oligomers of the Alzheimer peptide Abeta16-22: From the dimer to the 32-mer* 2006 **Biophysical Journal** 91 3217

47. Bussi, G., Gervasio, F.L., Laio, A., Parrinello, M. *Free-energy landscape for Î_ hairpin folding from combined parallel tempering and metadynamics* 2006 **Journal of the American Chemical Society** 128 13435

48. Park, J.M., Laio, A., Iannuzzi, M., Parrinello, M. *Dissociation mechanism of acetic acid in water* 2006 **Journal of the American Chemical Society** 128 11318

49. Zipoli, F., Laino, T., Laio, A., Bernasconi, M., Parrinello, M. *A QUICKSTEP-based quantum mechanics/molecular mechanics approach for silica* 2006 **Journal of Chemical Physics** 124 154707

50. Hugosson, H.W., Laio, A., Maurer, P., Rothlisberger, U. **A comparative theoretical study of dipeptide solvation in water** 2006 *Journal of Computational Chemistry* 27 672

51. Bussi, G., Laio, A., Parrinello, M. *Equilibrium free energies from nonequilibrium metadynamics* 2006 **Physical Review Letters** 96 90601

52. Raiteri, P., Laio, A., Gervasio, F.L., Micheletti, C., Parrinello, M. *Efficient reconstruction of complex free energy landscapes by multiple walkers metadynamics* 2006 **Journal of Physical Chemistry B** 110 3533

53. Laio, A., Micheletti, C. *Are structural biases at protein termini a signature of vectorial folding?* 2006 **Proteins: Structure, Function and Genetics** 62 17

54. Oganov, A.R., Martonak, R., Laio, A., Raiteri, P., Parrinello, M. *Anisotropy of earth's D"_ layer and stacking faults in the MgSiO 3 post-perovskite phase* 2005 **Nature** 438 1142

55. Laino, T., Mohamed, F., Laio, A., Parrinello, M. *An efficient real space multigrid QM/MM electrostatic coupling* 2005 **Journal of Chemical Theory and Computation** 1 1176

56. Sulpizi, M., Rothlisberger, U., Laio, A. *Electron transfer induced dissociation of chloro-cyano-benzene radical anion: Driving chemical reactions via charge restraints* 2005 **Journal of Theoretical and Computational Chemistry** 4 985

57. Zipoli, F., Bernasconi, M., Laio, A. *Ab initio simulations of Lewis-acid-catalyzed hydrosilylation of alkynes* 2005 **ChemPhysChem** 6 1772

58. Martonak, R., Laio, A., Bernasconi, M., Ceriani, C., Raiteri, P., Zipoli, F., Parrinello, M. *Simulation of structural phase transitions by metadynamics* 2005 **Zeitschrift fur Kristallographie** 220 489

59. Gervasio, F.L., Laio, A., Parrinello, M., Boero, M. *Charge localization in DNA fibers* 2005 **Physical Review Letters** 94 158103

60. Laio, A., Rodriguez-Fortea, A., Gervasio, F.L., Ceccarelli, M., Parrinello, M. *Assessing the accuracy of metadynamics* 2005 **Journal of Physical Chemistry** B 109 6714

61. Ensing, B., Laio, A., Parrinello, M., Klein, M.L. *A recipe for the computation of the free energy barrier and the lowest free energy path of concerted reactions* 2005 **Journal of Physical Chemistry B** 109 6676

62. Gervasio, F.L., Laio, A., Parrinello, M. *Flexible docking in solution using metadynamics* 2005 **Journal of the American Chemical Society** 127 2600

63. Roehrig, U.F., Guidoni, L., Laio, A., Frank, I., Rothlisberger, U. *A molecular spring for vision* 2004 **Journal of the American Chemical Society** 126 15328

64. Stirling, A., Iannuzzi, M., Laio, A., Parrinello, M. *Azulene-to-naphthalene rearrangement: The Car-Parrinello metadynamics method explores various reaction mechanisms* 2004 **ChemPhysChem** 5 1558

65. Gervasio, F.L., Laio, A., Iannuzzi, M., Parrinello, M. *Influence of DNA structure on the reactivity of the guanine radical cation* 2004 **Chemistry - A European Journal** 10 4846

66. Ceriani, C., Laio, A., Fois, E., Gamba, A., Martonak, R., Parrinello, M. *Molecular dynamics simulation of reconstructive phase transitions on an anhydrous zeolite* 2004 **Physical Review B** 70 113403

67. Raiteri, P., Laio, A., Parrinello, M. *Correlations among hydrogen bonds in liquid water* 2004 **Physical Review Letters** 93 87801

68. Ensing, B., Laio, A., Gervasio, F.L., Parrinello, M., Klein, M.L. *A minimum free energy reaction path for the E2 reaction between fluoro ethane and a fluoride ion* 2004 **Journal of the American Chemical Society** 126 9492

69. Ceccarelli, M., Danelon, C., Laio, A., Parrinello, M. *Microscopic mechanism of antibiotics translocation through a porin* 2004 **Biophysical Journal** 87 58

70. Laio, A., Gervasio, F.L., Vande Vondele, J., Sulpizi, M., Rothlisberger, U. *A variational definition of electrostatic potential derived charges* 2004 **Journal of Physical Chemistry B** 108 7963

71. Micheletti, C., Laio, A., Parrinello, M. *Reconstructing the density of states by history-dependent metadynamics* 2004 **Physical Review Letters** 92 170601

72. Roehrig, U.F., Frank, I., Hutter, J., Laio, A., VandeVondele, J., Rothlisberger, U. *QM/MM*

Car-Parrinello Molecular Dynamics Study of the Solvent Effects on the Ground State and on the First Excited Singlet State of Acetone in Water 2003 **ChemPhysChem** 4 1177

73. Sulpizi, M., Laio, A., VandeVondele, J., Cattaneo, A., Rothlisberger, U., Carloni, P. *Reaction mechanism of caspases: Insights from QM/MM Car-Parrinello simulations* 2003 **Proteins: Structure, Function and Genetics** 52 212

74. Iannuzzi, M., Laio, A., Parrinello, M. *Efficient exploration of reactive potential energy surfaces using car-parrinello molecular dynamics* 2003 **Physical Review Letters** 90 238302

75. Magistrato, A., DeGrado, W.F., Laio, A., Rothlisberger, U., VandeVondele, J., Klein, M.L. *Characterization of the dizinc analogue of the synthetic diiron protein DF1 using ab initio and hybrid quantum/classical molecular dynamics simulations* 2003 **Journal of Physical Chemistry B** 107 4182

76. Martonak, R., Laio, A., Parrinello, M. *Predicting crystal structures: The Parrinello-Rahman method revisited* 2003 **Physical Review Letters** 90 075503/1

77. Laio, A., Parrinello, M. *Escaping free-energy minima* 2002 **Proceedings of theNational Academy of Sciences of the United States of America** 99 12562

78. Colombo, M.C., Guidoni, L., Laio, A., Magistrato, A., Maurer, P., Piana, S., Roehrig, U., Spiegel, K., Sulpizi, M., VandeVondele, J., Zumstein, M., Rothlisberger, U. *Hybrid QM/MM Car-Parrinello simulations of catalytic and enzymatic reactions* 2002 **Chimia** 56 13

79. Laio, A., VandeVondele, J., Rothlisberger, U. D-RESP: *Dynamically generated electrostatic potential derived charges from quantum mechanics/molecular mechanics simulations* 2002 **Journal of Physical Chemistry** B 106 7300

80. Laio, A., VandeVondele, J., Rothlisberger, U. *A Hamiltonian electrostatic coupling scheme for hybrid Car-Parrinello molecular dynamics simulations* 2002 **Journal of Chemical Physics** 116 6941

81. Orlandini, E., Seno, F., Banavar, J.R., Laio, A., Maritan, A. *Deciphering the folding kinetics of transmembrane helical proteins* 2000 **Proceedings of the National Academy of Sciences of the United States of America** 97 14229

82. Laio, A. Bernard S. Chiarotti G., Scandolo S., Tosatti E., *Physics of iron at earth's core conditions* 2000 **Science** 287, 1027

83. Laio, A., Torre, V. *Physical origin of selectivity in ionic channels of biological membranes* 1999 **Biophysical Journal** 76 ,129

84. Laio, A., Santoro, G., Tosatti, E. *Interacting hard-core bosons and surface preroughening* 1998 Physical Review B 58, 13151

85. Santoro, G., Laio, A., Tosatti, E. *Step-step interactions and correlations from 1D hard-core boson mapping* 1998 **Surface Science** 402, 880

86. Santoro, G., Laio, A., Fabrizio, M., Tosatti, E. *Interacting hard-core bosons and surface physics* 1997 **Surface Science** 377, 514

87. Laio, A., Rizzi, G., Tartaglia, A. *Quantum theory of frequency shifts of an electromagnetic wave interacting with a plasma* 1996 **Physical Review E** 55, 7457

88. Accardi, L., Laio, A., Lu, Y.G., Rizzi, G. *A third hypothesis on the origin of the redshift: Application to the Pioneer 6 data* 1995 **Physics Letters A** 209 277

Teaching

Since 2006 I am holding at SISSA the course *Advanced sampling techniques for numerical simulations*, in which the most recent techniques for simulating rare events, exploring the phase space and computing the free energy are summarized. In October-December 2008 I held the same course at the University College London.

Invited Lectures

I here list the invited lectures in international conferences and workshops I gave in the last ten years. In the same period, I was also invited by more than 40 institutions and research groups to give named seminars.

- **RARE2014: Recent advances in modeling rare events,** 29 May-2 June 2014, Kerala (India)
- **Advanced modeling to investigate biomolecules**, 20-21 November, Genova (Italy)
- **New Approaches in Materials Design**. 11-12 December 2014, Moscow (Russia).
- **Advanced School on Synchrotron Radiation Techniques and Nanotechnology: A Synergic Approach to Life Sciences and Medicine**, 11-22 November 2013, Cape Town (South Africa)
- **Modelling the Dynamics of Complex Molecular Systems,** 27-31 August 2012, Leiden (Netherlands)
- **Molecular Structure, Dynamics and Recognition of Biomolecules,** June 5-6, 2012 , Tel Aviv (Israel)
- **Berkeley Statistical Mechanics Meeting,** January 13-15, 2012 (Berkeley, USA)
- **International Conference on Statistical Physics SigmaPhi2011,** 11-15 July 2011 Larnaka, (Cyprus)
- **Beyond Molecular Dynamics : Long time scale atomistic simulation,,** March 26-29 2011, Dresden (Germany)

- **Fall symposium of the Amsterdam Center for Multiscale Modeling,** 18-19 November 2010, Amsterdam (Netherlands)
- **CECAM Workshop on Protein Folding,** Oct 4-7 2010, Lausanne (Switzerland)
- **Multiscale Molecular Modelling: Molecular Dynamics, Computational Statistical Mechanics, and Simulation Algorithms,** June 28-July 2, 2010, Edinburgh (UK)
- **Molecular Kinetics 2009,** May 25-29 2009 (Berlin)
- **Accessing large length and time scales with accurate quantum methods,** 12-13 January 2009, London (UK)
- **DFT09,** 31 August-4 September 2009, Lyon (France)
- **Metastability and Rare Events in complex Systems,** 18-22 February 2008, Wien (Austria)
- **1st Intl Conference of the Grand Challenge to Next Generation Integrated Nanoscience,** 3-6 June 2008, Tokyo (Japan)
- **Workshop on long time dynamics,** 16-17 April 2007, Loughborough (UK)
- **Frontiers in mineralogy,** 26-28 June 2007, Cambridge (UK)
- **Molecular Modelling 2006,** 19-22 April 2006, Perth (Australia)
- **Asian Workshop on First-Principles Electronic Structure Calculations** 31 October - 2 November 2005, Shanghai (China).
- **Computer Simulations in Condensed Matter: from Materials to Chemical Biology,** 20-31 July 2005, Erice (Italy).
- **Matter, Materials and Devices Meeting,** 21-24 June 2005, Genova (Italy).
- **CECAM Workshop on First-Principles Simulations: Perspectives and Challenges in Mineral Sciences,** 27 September- 1 October 2004, Lyon (France).
- **CECAM Workshop on Conformational Dynamics in Complex Systems,** 12-23 August 2004, Lyon (France).
- **Third Stig Lundqvist Conference on Advancing Frontiers in Condensed Matter Physics,** 11-15 August 2003, Trieste (Italy).
- **XI International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods,** 16-18 January 2003, Trieste (Italy).
- **Joint 33rd Speedup and 19th PARS Workshop,** 19 March 2003, Basel

(Switzerland).

- **CECAM Workshop on Reactive Classical Potentials versus Hybrid Methods: Toward Chemical Complexity,** June 16-19, 2003 Lyon (France).

Trieste, 13/1/2014