

Prof. Francesco Sciortino. Curriculum Vitae atque Studiorum.

Scientific Profile

I have started my scientific career as Ph.D. student in Palermo in 1985 in the group of Prof. M.U. Palma, focusing on the phase behavior of biopolymers in solution. I used dynamic light scattering methods to evaluate structural and thermodynamic changes in the system as a function of temperature and concentration. The results were reported in two articles, published in *Biopolymers*. In the same years, in the process of deepening my knowledge about hydrophobic and hydrophilic interactions, I started to study the physical properties of water in detail. I was very much impressed by a study on percolation theory applied to water, by J. Teixeira and H.E. Stanley, which had recently appeared. To test some new ideas on how to quantify the connectivity of hydrogen bonds in water, I decided to complement my experimental activity with some direct experience in the field of numerical simulations. Prof. S. Fornili offered me a tape with a 20 ps trajectory of water molecules which I analyzed in an original way, discovering a correlation in the special distribution of hydrogen bonds. Thanks to this work, published in *J. Chem. Phys.*, I was offered a Post-Doc position at Boston University in the group of Prof. H.E. Stanley, where I moved in 1989.

The two and a half years I have spent in Boston have strongly affected my career. While investigating the behavior of super-cooled water I personally came up with a completely new way of looking at the thermodynamic anomalies characteristic of water (density maxima, compressibility minima). I suggested the possibility of a new thermodynamic scenario: the existence of a second critical point in the liquid phase located in the so-called no-man's land, i.e. below crystallization. This idea, which has been tested in numerical simulations performed by the Ph.D student P. Poole, appeared in *Nature*. My idea has generated an extensive experimental and theoretical activity due to the possibility of interpreting in a novel paradigm not only the properties of water as a pure liquid, but also the properties of water as biological solvent. I also proposed a structural mechanism for explaining the mobility of water and the (counterintuitive) speeding up of the dynamics on compression. This work has been published in *Nature*. During the post-doc years, I have also participated to one of the first statistical analysis of the DNA sequences, discovering interesting differences between coding and non-coding parts of the DNA. Also this work has appeared in *Nature*. Besides being exposed to an exciting research environment and to several new fields, while in Boston I started to learn how to guide scientific research in an efficient way. Indeed, Prof. H.E. Stanley offered me to supervise three of his Ph.D. students (S. Sastry, P. Poole, S. Glotzer), all of them nowadays well established university professors. I continued to collaborate with Prof. Stanley for more than ten years, following the Ph.D. research of several of his students (F. Starr, S. Harrington, Y. Masako, N. Giovambattista, E. La Nave, A. Scala, P. Kumar).

After leaving Boston and a short-intermediary period at CRS4 in Sardinia (in the group of Prof. E. Clementi), I moved to University of Roma La Sapienza as Ricercatore (assistant professor) first in the group of Prof. Tartaglia and then, after becoming associate professor, building my own group. My move to the University of Roma coincided with the opening of a new research field, the slowing down of the molecular dynamics on approaching the glass transition. It has been a very rich and productive time. Computers had just reached the ability to generate trajectories covering several orders of magnitude in time, offering for the first time the possibility to closely test available theoretical predictions. In particular I focused on the mode coupling theory (MCT) developed by W. Goetze and coworkers and compared the theoretical predictions with 100 ns long simulations of supercooled water and orthoterphenyl. This test of the theory, shortly following the analog study done by W. Kob for Lennard-Jones particles. In the attempt to provide closer test between theoretical predictions and numerical simulations, and despite the amazing complexity of the equations, I collaborated with Prof. Schilling in testing, for the first time, the molecular version of the MCT. Besides the MCT analysis, I also focused on a thermodynamic approach to the glass transition based on the potential energy land-

scape (PEL) formalism. In this respect, I consider particularly relevant two contributions of mine: (1) The evaluation (after deriving the correct methodology) of the inherent structure entropy of super-cooled liquids (a manuscript published in PRL in 1999). The new methodology has offered for the first time the possibility of estimating numerically the configurational entropy, a quantity previously approximated postulating the equivalence between vibrational properties of the crystal and of the corresponding glass. This methodology has been successfully applied to several models. Particularly relevant has been the investigation of the correlation between configurational entropy and diffusivity in water (with Prof. Stanley) and silica (with Prof. Poole). Both studies have appeared in *Nature*. (2) The first precise PEL theoretical evaluation (and numerical confirmation) of the effective temperature during aging.

In the last years, I have transferred the know-how developed in the study of glass forming molecular liquids to tackle the problems of arrested states in colloidal systems. A significant achievement has been the discovery, based on MCT calculations and confirmed in numerical simulations, of a re-entrant glass formation in short-range attractive colloidal systems. This discovery (resulting from a collaboration with W. Goetze) has been reported in two highly cited Phys. Rev. E articles and commented in a News and Views article written by me in *Nature Materials* in 2002, in occasion of the experimental verification of the theoretical and numerical predictions.

From glasses to gels could be the title of my most recent step forward. I have realized that colloidal gelation in the presence of electrostatic repulsions and short-range attraction may lead to a suppression of a macroscopic thermodynamic instability and to the formation of cluster phases and macroscopic gels. Even more recently, I have discovered that the reduction of the valence provides also an interesting mechanism for suppressing phase separation and stabilizing equilibrium gel phases. In the very last years, I have started to focus on the interplay between phase separation and self-assembly in colloidal systems.

I could not have done all this work without the help of students and collaborators. For several years, I have continued to collaborate with Prof. H.E. Stanley group (with a visiting scientist position), following the Ph.D. research of many students. Many of these researches have produced innovative and well received articles. At the same time, I have followed in Roma the Laurea research of sixteen students and the Ph.D. research of five students. Several of them continue their research activity. Finally, despite the known difficulties for Italy, I have attracted several foreigner post-docs in my group, among which S.H. Chong, I. Saika-Voivod, A. Moreno, J. Largo, C. Mayer, F. Smallberger, T. Visser, S. Roldan. Several of them have now positions in Universities or research centers. Finally, I had (and still have!) the pleasure to collaborate with several leading scientists, which can be easily identified from the co-author list. I am proud of having been able to build a human and scientific network which includes so many outstanding scientists as nodes. The pleasure to discuss science with them and to unravel the truly controversial issues has been and will continue to be an important part of my activities.

Short Biography

born in Palermo (Italy), December 29, 1960.

- 1984 Laurea cum laude in Physics, Università degli Studi di Palermo. Thesis: Transizione-Ordine - Disordine topologico in un sistema biostrutturale: studio degli effetti di un rumore dicotomo di Markov sul processo di ordinamento sovramolecolare. (Order-Disorder topological transition in a biostructural system. Study of the effect of a Markov dichotomous noise on a supramolecular ordering process).
- 1989 Ph.D. Thesis, Università degli Studi di Palermo: Il sistema accoppiato biomolecole-solvente: Meccanismi cooperativi nell'hydrogen bonding e ruolo delle instabilità

termodinamiche nei processi di ordinamento sovramolecolare. (The coupled solvent-biomolecule system: cooperative mechanisms in the hydrogen bonding and role of the thermodynamic instabilities in supramolecular ordering processes).

- 1989-1991 Post-doctoral fellow - Boston University (BU), Center for Polymer Studies, in the group of prof. H.E. Stanley.
- 1992 Researcher C.R.S.4, Centro Ricerche, Sviluppo, Studi Superiori in Sardegna, Cagliari (Group Prof. Clementi).
- 1992-2003 Visiting Research Associate, Boston University, Center for Polymer Studies (Prof. H.E. Stanley).
- Sept. 1995 Maitre de Conference, Université de Bordeaux I
- 1993-2000 Assistant Professor, Università di Roma La Sapienza.
- May 2000 Visiting Professor, Université de Bordeaux I
- 2001-2004 Associate Professor, Università di Roma La Sapienza.
- June 2004 Visiting Professor, University of Western Ontario, Canada.
- 2005-today Full Professor, Università di Roma La Sapienza.

Research interests:

- Self assembly in colloidal systems and protein solutions, bio-functionalized colloids.
- Aggregation phenomena in colloidal systems, cluster phases and gels.
- Thermodynamics of anomalous liquids, multiple critical points.
- Glass transition in super-cooled liquids. Aging phenomena.
- Percolation and phase transitions in complex fluids.
- Thermodynamics of super-cooled liquids. Potential energy landscape formalism.

International collaborations: I had and I still have the pleasure to collaborate with several leading scientists and with their students. A list of the senior scientists includes: A. Angell (Arizona State U.), P. De Benedetti (Princeton U.), S.H. Chen (MIT), J. Douglas (NIST), W. Goetze (Munich T.U.), W. Kob (U. Montpellier), C. Likos (Duesseldorf U.), H. Loewen (Duesseldorf U.), P. Poole (St. Francis Xavier University), S. Sastry (JNC Bangalore), R. Schilling (U. Mainz), P. Schurtenberger (Friburg), H.E. Stanley (Boston U.), F. Starr (Wesleyan U.), D. Weitz (Harvard U.), M. Telo da Gama (Lisboa University), S. Kumar (Columbia).

Editorial Activities: Member of the Editorial Board of *Chemical Physics* (2001-2004). Member of the Editorial Board of *J. Phys. Condensed Matter* (2003-2007) Since January 2008, Editor of the *Liquids and Biological Physics* section of *J. Phys. Condensed Matter*.

Other Activities: (2002-2003) Member of the ESRF review committee. (2007-2012) Member of the Liquid Board of the European Physical Society. (2009-2011) Director of SOFT (I was Deputy director between 2004-2008). SOFT is a CRS (Centro di Ricerca e Sviluppo) of INFM (Istituto Nazionale Fisica della Materia) (now INFM-CNR) devoted to the investigation of the complex dynamics in structured systems (<http://www.crs-soft.it/index.html>). This center was created on the basis of a project presented to INFM by Prof. Giancarlo Ruocco and myself. (2005-2010) Member of the scientific committee of the Erasmus Mundus ATOSIM program. ATOSIM is a one year Physics and

Chemistry masters degree focused on computer modelling of physical, chemical and biomolecular systems.

Referee for National Science Foundation (USA), Austrian Science Fund, NSERC (Canada). Referee for several journals including JPCM, EPL, ACS Journals, APS Journals, Soft Matter, *Nature*, *Nature Materials*.

Educational Activity: Supervisor of several *Laurea* students (P. Finocchi, E. La Nave, C. Padoa Schioppa, L. Rosso, F. Thiery, P. Laureti, E. Zaccarelli, G. Foffi, A. Rinaldi, C. Valeriani, E. Bianchi, S. Gabrielli, F. Ciulla, F. Romano, Z. Slimani, O. Akinde, S. Dussi) and Ph.D. students (L. Fabbian, N. Ghofraniha, E. Bianchi, J. Russo, F. Romano, S. Rovigatti, F. Bomboi, N. Thuy, G. Das, Z. Pressler). Mentor of post-docs (S.H. Chong, C. Donati, C. De Michele, G. Foffi, E. La Nave, J. Largo, C. Mayer, A. Moreno, S. Mossa, I. Saika-Voivod, A. Scala, E. Zaccarelli, N. Gnan, G. Munao, T. Visser, S. Roldan, F. Smallenburg).

In the last 10 years I have been invited to speak in more than 40 conferences, listed in <http://glass.phys.uniroma1.it/sciortino/talks.htm>. The list includes Material Research Society meetings, StatPhys 2007, the International Soft Matter Conference 2007, American Chemical Society meeting years 1999, 2001, 2002, 2007, American Physical Society meeting 2002, Gordon Conference 1999, 2002 and 2012, the European Liquid Matter Conference 2002. I list here only a few of them here to provide an evidence of the different problems I have been working in my career:

(*)GRC Ventura 2012, Patchy colloid (gels) phase diagrams. (*)Complex transport in strongly interacting systems, Munich, Re-entrant phase behavior of network fluids: A patchy particle model with temperature-dependent valence. (*) MRS 2011 Boston, Colloidal Gels: Insight from Numerical Studies. (*) Liblice 2010, Self Assembly of patchy particles. (*) Lisbon 2009, Flow(ers) and Jam(mers), Gel-forming patchy colloids. (*) Cecam, Losanne 2009, Phase Diagram of Janus Particles. (*) SIBPA, Roma, Some possible connections between the physics of colloids and of proteins. (*) XXI Sitges Conference 2008, Self Assembly of Patchy Particles and DNA-Functionalized Dendrimers (*) International Soft Matter Conference, Aachen, (2007), Patchy colloidal particles: the role of the valence in the formation of gels. (*) StatPhys 23 Genova (2007), Gel-forming patchy colloids and network glassformers: Thermodynamic and Dynamic analogies (*) ACS March Meeting Chicago (2007), Gel-forming patchy colloids, and network glass formers: Thermodynamic and dynamic analogies (*) Marie Curie Workshop on Dynamical arrest of soft matter and colloids. Lugano (2005), Tutorial: Recent developments in understanding gelation in colloidal systems (*) 5th IDM-RCS Lille (2005) Statistical properties of the landscape of a simple strong liquid model and something else. (*) Networks in physics and biology Orleans (2004) Potential Energy Landscape in Models for Liquids (*) 5th Liquid Matter Conference, Konstanz. (2002), Potential Energy Landscape Equation of State. (*) Gordon Research Conference Water and aqueous solutions Holderness (2002), Water and its energy landscape. (*) American Physical Society, Indianapolis, (2002) Energy Landscape in supercooled liquids (*) ESF Molecular Liquids: Obernai, (2001). Supercooled water dynamics: Normal or anomalous behaviour ? (*) ACS San Diego (2001), Thermodynamics and Aging of Supercooled Liquids: The energy landscape approach (*) European Physical Society meeting: Montreaux (2000) Aging as dynamics in configuration space (*) ERC Molecular Liquids, San Feliu de Guixols, (1999) Instantaneous Normal Mode Approach to the dynamics of water (*) American Chemical Society, New Orleans (1999), Slow Dynamics in Supercooled Water: Theory and Simulations (*) Gordon Research Conference Water and aqueous solutions Holderness (1998) Dynamics of Supercooled Water: A theoretical description.

Seminars: The universities, in Italy, where I have been invited to deliver talks include Messina, Firenze, Aquila, Perugia, Trieste, Milano, Palermo, Pisa, Padova. In Europe, I have presented my work in Vienna (G. Kahl), Duesseldorf (H. Loewen), Amsterdam (D. Frenkel), Cambridge (J.P. Hansen), Cambridge (Eiser, Frenkel), Montpellier (W. Kob), Munich (W. Goetze), Mainz (K. Binder), Kohl (J. Horbach), Lisbon (da Gama), Madrid (Vega). Overseas, I have delivered talks in Michigan

U. (S. Glotzer), Columbia U. (S. Kumar), Princeton U. (P. De Benedetti), MIT (S.H. Chen), Boston U. (H.E. Stanley), NIST (S. Glotzer)

Organization of international conferences: In the last years I have been: (*) co-organizer (with P. Madden and T. Keyes) CECAM workshop The Instantaneous Normal Mode Approach to Dynamics in Liquids, 1999 Lyon. (*) Co-organizer (with A. Crisanti, E. Marinari and G. Parisi) International conference Unifying concepts in the glass transition II Roma, 2002. (*) Co-organizer (with S.H. Chen and F. Mallamace) workshop Short range attractive colloidal systems, Messina, 2004. (*) Co-organizer (with E. Zaccarelli) CECAM workshop Patchy Colloids, Proteins and Network-Forming Liquids, Lyon 2006 (*) Coorganizer (with C. Likos) Soft, Complex, and Biological Matter Conference, 2007, Cinisi. (*) Co-organizer (with M. Solomon) of the symposium Colloidal Glasses and Gels, 81st Colloid and Surface Science ACS, 2007, Newark, Delaware (*) Co-organizer (with E. Luijten and S. C. Glotzer) of the symposium on Design, Fabrication and Self-Assembly of Patchy and Anisometric Particles, MRS 2008 Boston. (*) Co-organizer (with I. Coluzza, C. Dellago and J. Dobnikar) CECAM workshop, Design of self-assembling materials, Vienna 2012. (*) Chairman of the International Soft Matter Conference, to be held in Roma, September 15-19 (2013). (*) Director (with C. Bechinger and P. Ziher) of the CLXXXIV Varenna School on the Physics of Complex Colloids, attended by 65 students (July 2012). I have been (*) Member of the International program committee for the International Workshop on Dynamics in Viscous Liquids, Munich 2004. (*) Member of the International program committee for the 7th EPS Liquid Matter Conference, Lund 2008; (*) Member of the International program committee for the III and IV international conference Unifying concepts in the glass transition, Bangalore (2004) and Kyoto (2008). (*) Member of the International program committee of StatPhys, Melburn (2010). (*) Member of the International program committee for the 8th EPS Liquid Matter Conference, Vienna (2011).;

Lecture Notes, Review Articles, News and Views

F. Sciortino, Potential energy landscape description of supercooled liquids and glasses J. Stat. Mech. 050515, 2005. Lecture notes of the ICTP/JNC school Unifying concepts in glass physics III Franz S. and S. Sastry (eds).

F. Sciortino and P. Tartaglia, Glassy colloidal systems, Advances in Physics 54, 471-524, 2005

F. Sciortino Disordered materials: one liquid, two glasses, News and Views, Nature Materials 1, 145-146, 2002

F. Romano and F. Sciortino, Patchy from the bottom, Nature Materials, News and Views, 10, 171 (2011)

Francesco Sciortino, Silicon in silico, Nature Physics, News and Views, 7, 523-524 (2011).

Francesco Sciortino, Viewpoint: DNA Hairs Provide Potential for Molecular Self-Assembly Physics 5, 71 (2012)

Recent funding: I have constantly applied for grants from the Italian Ministry of the University (MIUR) with very good success. I have been funded with PRIN-type projects in 2001-2002, 2003-2004, 2006-2007 and 2011-2013. Since year 2001, I have always been the National coordinator of the project, coordinating several research units distributed all over Italy. The total grant value is of the order of 200-300 keuro for year. I have also received a MIUR-FIRB-type grant, entitled *Short-range attractive colloids: models for protein crystallization* (557 keuro) covering the period 2002-2005. I am the scientist in charge of the Roma node of the Marie Curie-Initial Training Network "Physics of Complex Colloids: Equilibrium and Driven (ITN-COMPLOIDS)", funded with 300 keuro. In 2010 I was awarded a ERC Senior Grant PATCHYCOLLOIDS for 1500 keuro to investigate the phase behavior of new generation colloids.

Publications: I am author of more than 330 publications in international journals. I have coauthored 47 articles which have appeared in Phys. Rev. Lett., 6 which have been published in *Nature* and

three in *Nature Materials* . Thirty-four have received more than 100 citations. I have received a total number of citations larger than 13200, of which 1200 during 2011. My h-index (Oct 2011) is 59. The complete list of publications is available at <http://glass.phys.uniroma1.it/sciortino/publications.htm>

Some Relevant Publications

- 1 Sciortino F, Geiger A, Stanley H.E. Effect of Defects on molecular mobility in liquid water, *Nature* 354 218-221 (1991). Times Cited 212.
- 2 Poole, P.H., Sciortino F., Essmann U. Stanley H.E., Phase Behavior of metastable water, *Nature*, 360, 324-328 (1992). Times Cited 752.
- 3 Sciortino, F; Gallo, P; Tartaglia, P. and Chen S.H., Supercooled water and the kinetic glass transition, *Phys. Rev. E*, 54, 6331-6343 (1996). Times Cited 232.
- 4 Sciortino F, Kob W, Tartaglia P, Inherent structure entropy of supercooled liquids, *Phys. Rev. Lett.*, 83, 3214 (1999). Times Cited: 289
- 5 Scala A, Starr FW, La Nave E, Sciortino F, Stanley H.E., Configurational entropy and diffusivity of supercooled water *Nature* 406 166 (2000). Times Cited: 220
- 6 Saika-Voivod I, Poole P.H, Sciortino F, Fragile-to-strong transition and polyamorphism in the energy landscape of liquid silica, *Nature*, 412 514 (2001). Times Cited: 190
- 7 Sciortino F and Tartaglia P, Extension of the fluctuation-dissipation theorem to the physical aging of a model glass-forming liquid *Phys. Rev. Lett.* 86 107 (2001). Times Cited: 105
- 8 La Nave E, Mossa S, Sciortino F, Potential energy landscape equation of state *Phys. Rev. Lett.* 88, 225701 (2002). Times Cited: 59
- 9 Sciortino F, Disordered materials - One liquid, two glasses, *Nature Materials, News and Views*, 1, 145-146 (2002) Times Cited: 92.
- 10 Sciortino F, Mossa S, Zaccarelli E and Tartaglia P., Equilibrium cluster phases and low-density arrested disordered states: The role of short-range attraction and long-range repulsion *Phys. Rev. Lett.* 93, 055701 (2004). Times Cited: 205
- 11 Bianchi E, Largo J, Tartaglia P, Zaccarelli E. and Sciortino F., Phase diagram of patchy colloids: Towards empty liquids *Phys. Rev. Lett.* 97 168301 (2006). Times Cited: 150
- 12 Lu, Peter J.; Zaccarelli, Emanuela; Ciulla, Fabio; Sciortino F. Weitz D. Gelation of particles with short-range attraction, *Nature* 453 499 (2008). Times Cited 204.
- 13 Hsu, Chia Wei; Largo, Julio; Sciortino, Francesco, Starr Francis, Hierarchies of networked phases induced by multiple liquid-liquid critical points, *Proceedings National Academy of Sciences*, 105, 13711-13715 (2008). Times Cited 23.
- 14 Sciortino, Francesco; Giacometti, Achille; Pastore, Giorgio, Phase Diagram of Janus Particles, *Phys. Rev. Lett.* 103, 237801 (2009). Times Cited: 50
- 15 Russo, J.; Tavares, J. M.; Teixeira, P. I. C., Telo da Gama M, Sciortino F, Reentrant Phase Diagram of Network Fluids, *Phys. Rev. Lett.* 106 085703 (2011). Times Cited 18.