

PART I  
GENERAL INFORMATION



## Cristiano De Michele

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Spoken Languages: Italian (mother tongue), English (fluent) and French (basic)

PART II  
EDUCATION

05/12/17 **Abilitazione Scientifica Nazionale (National Scientific Qualification)**

come Professore di **Prima Fascia** (as Full Professor)

in Fisica Teorica della Materia (02/B2 – Theoretical Condensed Matter Physics)

05/12/17 **Abilitazione Scientifica Nazionale (National Scientific Qualification)**

come Professore di **Seconda Fascia** (as Associate Professor)

in Fisica Teorica della Materia (02/B2 – Theoretical Condensed Matter Physics)

11/12/13 **Abilitazione Scientifica Nazionale (National Scientific Qualification)**

come Professore di **Seconda Fascia** (as Associate Professor)

in Fisica Teorica della Materia (02/B2 – Theoretical Condensed Matter Physics)

22/12/03 **PhD in "Fundamental and Applied Physics"**

University of Naples "Federico II"

thesis title "Fragility in Soft Sphere Systems: Role of the Repulsive Potential"

supervisor Prof. Antonio Coniglio

17/03/98 **Master in Physics**

University of Pisa

final mark 110/110 cum laude supervisor Prof. Dino Leporini

01/07/92 **High School Degree**

Liceo Scientifico "R. Donatelli" - Terni

final mark 60/60

PART III  
ACADEMIC APPOINTMENTS

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March 2020	<b>Associate Professor (Professore di II fascia)</b> Department of Physics, "Sapienza", University of Rome
March 2017-February 2020	<b>Tenure-track Associate Professor (RTDb - art. 24 c.3-b L. 240/10)</b> Department of Physics, "Sapienza", University of Rome
December 2015 - February 2017	<b>Non-tenure Assistant Professor <b>part-time</b> (RTDa - art. 24 c.3-a L. 240/10)</b> Department of Physics, "Sapienza", University of Rome
December 2015 - present	<b>1 year position as research fellow <b>part-time</b></b> Centre de Biophysique Moléculaire (CBM) of CNRS, Orleans, France. Thanks to an <b>award</b> from Loire Valley Institute for Advanced Studies, Orleans, France ( <a href="http://www.lestudium-ias.com/">http://www.lestudium-ias.com/</a> )
December 2012 - November 2015	<b>Non-tenure Assistant Professor (RTDa - art. 24 c.3-a L. 240/10)</b> Department of Physics, "Sapienza", University of Rome
December 2009 - November 2012	<b>Non-tenure Assistant Professor (RTD - art.1 comma 14 L. 230/05)</b> Department of Physics, "Sapienza", University of Rome
October 2008 - September 2009	<b>Postdoctoral Research Fellowship</b> Department of Physics, "Sapienza" University of Rome Supervisor: Prof. Giovanni Ciccotti
May 2008 - September 2008	<b>Postdoctoral Scholarship</b> Department of Physics, "Sapienza" University of Rome Supervisor: Prof. Francesco Sciortino
May 2008 - July 2008	<b>Visiting Scientist</b> École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland Supervisor: Prof. Giuseppe Foffi
April 2008 - June 2008	<b>Postdoctoral Scholarship</b> CNR-INFM Laboratorio Regionale POLYLAB, Pisa Supervisor: Prof. Dino Leporini
January 2007 - December 2007	<b>Postdoctoral Scholarship</b> Department of Physics, "Sapienza" University of Rome Supervisor: Prof. Francesco Sciortino

- December 2006 - January 2007 **Visiting Scientist**  
 École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland  
 Supervisor: Prof. Giuseppe Foffi
- January 2006 - December 2006 **Postdoctoral Scholarship**  
 Department of Physics, "Sapienza" University of Rome  
 Supervisor: Prof. Francesco Sciortino
- January 2004 - December 2005 **Postdoctoral Research Fellowship (2 years)**  
 Department of Physics, "Sapienza" University of Rome  
 Supervisor: Prof. Francesco Sciortino
- April 1998 - May 1998 **Postgraduate Research Grant**  
 Department of Physics, University of Pisa  
 Supervisor: Prof. D. Leporini

#### PART IV TEACHING EXPERIENCE

- 2023-2024 **Lecturer (teacher in charge of the full course)**  
 Course: Computing Methods for Physics  
 60 hours  
 Laurea Magistrale in Fisica, "Sapienza" Università di Roma
- 2023-2024 **Lecturer (teacher in charge of the full course)**  
 Course: Laboratorio di Calcolo [1035105]  
 60 hours  
 Laurea Triennale in Fisica, "Sapienza" Università di Roma
- 2022-2023 **Lecturer (teacher in charge of the full course)**  
 Course: Computing Methods for Physics  
 60 hours  
 Laurea Magistrale in Fisica, "Sapienza" Università di Roma
- 2022-2023 **Lecturer (teacher in charge of the full course)**  
 Course: Laboratorio di Calcolo [1035105]  
 60 hours  
 Laurea Triennale in Fisica, "Sapienza" Università di Roma
- 2021-2022 **Lecturer (teacher in charge of the full course)**  
 Course: Computing Methods for Physics  
 60 hours  
 Laurea Magistrale in Fisica, "Sapienza" Università di Roma
- 2021-2022 **Lecturer (teacher in charge of the full course)**  
 Course: Laboratorio di Calcolo [1035105]  
 60 hours  
 Laurea Triennale in Fisica, "Sapienza" Università di Roma
- 2020-2021 **Lecturer (teacher in charge of the full course)**  
 Course: Computing Methods for Physics  
 60 hours  
 Laurea Magistrale in Fisica, "Sapienza" Università di Roma
- 2020-2021 **Lecturer (teacher in charge of the full course)**  
 Course: Laboratorio di Calcolo [1035105]  
 60 hours  
 Laurea Triennale in Fisica, "Sapienza" Università di Roma
- 2019-20 **Lecturer (teacher in charge of the full course)**  
 Course: Atomistic Simulations  
 60 hours  
 Laurea Magistrale in Fisica, "Sapienza" Università di Roma
- 2019-20 **Lecturer (teacher in charge of the full course)**  
 Course: Laboratorio di Calcolo [1035105]

- 60 hours  
Laurea Triennale in Fisica, "Sapienza" Università di Roma  
**2018-19 Lecturer (co-teaching)**  
Course: Laboratorio di Fisica Computazionale I [1012086]  
36 hours  
Laurea Triennale in Fisica, "Sapienza" Università di Roma  
**2018-19 Lecturer (co-teaching)**  
Course: Laboratorio di Calcolo [1035105]  
48 hours  
Laurea Triennale in Fisica, "Sapienza" Università di Roma  
**2017-18 Lecturer (teacher in charge of the full course)**  
Course: Simulazioni Atomistiche [1047781]  
60 hours  
Laurea Magistrale in Fisica, "Sapienza" Università di Roma  
**2017-18 Lecturer (laboratory teaching)**  
Course: Laboratorio di Calcolo [1035105]  
36 hours  
Laurea Triennale in Fisica, "Sapienza" Università di Roma  
**2016-17 Lecturer (teacher in charge of the full course)**  
Course: Fisica I [1015377]  
40 hours  
Laurea Triennale in Ingegneria Meccanica e in Ingegneria per l'Ambiente ed il Territorio, "Sapienza" Università di Roma  
**2016-17 Lecturer (teacher in charge of the full course)**  
Course: Fisica Generale [1052116]  
56 hours  
Laurea Triennale in Scienze Geologiche, Dipartimento di Scienza della Terra, "Sapienza" Università di Roma  
**2014-15 Lecturer (teacher in charge of the full course)**  
Course: Fisica Computazionale della Materia [1012139]  
60 hours  
Laurea Magistrale in Fisica, "Sapienza" Università di Roma  
**2013-14 Lecturer (teacher in charge of the full course)**  
Course: Fisica Computazionale della Materia [1012139]  
60 hours  
Laurea Magistrale in Fisica, "Sapienza" Università di Roma  
**2012-13 Lecturer (teacher in charge of the full course)**  
Course: Fisica Computazionale della Materia [1012139]  
60 hours  
Laurea Magistrale in Fisica, "Sapienza" Università di Roma  
**2011-12 Lecturer (teacher in charge of the full course)**  
Course: Fisica Computazionale della Materia [1012139]  
60 hours  
Laurea Magistrale in Fisica, "Sapienza" Università di Roma  
**2009-10 Teaching Assistant**  
Course: Fisica dei Liquidi  
Professor: P. Tartaglia  
Laurea Magistrale in Fisica, "Sapienza" Università di Roma  
**Teaching Assistant**  
Course: Fisica Computazionale della Materia  
Professor: P. Tartaglia  
Laurea Magistrale in Fisica, "Sapienza" Università di Roma  
**2007-2008 Teaching Assistant**  
Course: Laboratorio di Fisica Computazionale I  
Professor: A. Crisanti  
Laurea Triennale in Fisica, "Sapienza" Università di Roma  
**2006-2007 Teaching Assistant**  
Course: Laboratorio di Fisica Computazionale I  
Professor: A. Crisanti  
Laurea Triennale in Fisica, "Sapienza" Università di Roma

**2005-2006 Teaching Assistant**  
 Course: Laboratorio di Fisica Computazionale I  
 Professor: A. Crisanti  
 Laurea Triennale in Fisica, "Sapienza" Università di Roma

#### PART V AWARDS AND HONORS

**09/1992 Scholarship** in Physics at the **Scuola Normale Superiore di Pisa**  
 (posto ordinario nella Classe di Scienze della Scuola Normale)

**09/1992 "Elia Rossi Passavanti" award** for exceptional marks during high school.

#### PART VI FUNDING INFORMATION

I participated in many national and international projects as Investigator, such as several PRIN from MIUR (<http://print.miur.it>), n. 1 ERC-Advanced Grant (PI: Prof. Francesco Sciortino), several "Progetti di Ateneo" from "Sapienza" University of Rome and others. My grants as Principal Investigator are the following:

Event-driven simulations of primitive models in biological systems:  
antibody-antigen interaction.

**Swiss National Science Foundation (SNF) No. IZK022-121268**

01/04/2008 – 30/06/2008

**CHF 5.930**

Principal Investigator: Cristiano De Michele

Phase diagrams of colloidal suspensions: theory and simulations

**"Sapienza" Università di Roma**

**EUR 10.000**

01/01/2011-31/12/2011

Principal Investigator: Cristiano De Michele

Progetti di Ricerca 2010

Self-assembly of DNA duplexes into polymers chains: theory, simulations and experiments

**"Sapienza" Università di Roma**

**EUR 12.000**

01/01/2012-31/12/2012

Principal Investigator: Cristiano De Michele

Progetti di Ricerca 2011

Self-assembly of DNA duplexes into polymers chains: theory, simulations and experiments

**Jülich Supercomputing Centre (JSC) in Germany**

**1000 Tflops-hours**

01/01/2011 - 31/12/2011

Principal Investigator: Cristiano De Michele

DNA self-assembly

**"Sapienza" Università di Roma**

**EUR 40.000**

01/01/2013-31/12/2013

Principal Investigator: Cristiano De Michele

Progetti di Ricerca 2012

Conformation of short DNA duplexes

**Jülich Supercomputing Centre (JSC) in Germany**

**2700 Tflops-hours**

01/01/2013 - 31/12/2013

Principal Investigator: Cristiano De Michele

Theoretical models of complex nanostructured materials: ionic liquids from a coarse-grained perspective

**"Sapienza" Università di Roma****EUR 12.000**

01/01/2014-31/12/2014

Principal Investigator: Cristiano De Michele

Progetti di Ricerca 2013

Chiral Self-Assembly-Driven Liquid Crystals: Thermodynamic and Elastic Properties**"Sapienza" Università di Roma****EUR 13.800**

21/01/2017 - Prot. N. RM11715C639F6A69

Principal Investigator: Cristiano De Michele

Progetti di Ricerca 2017

Nanofabrication of Novel Liquid Crystals via DNA Self-Assembly**"Sapienza" Università di Roma****EUR 4.000**

11/12/2020 - Prot. N. RP120172B8851190

Principal Investigator: Cristiano De Michele

Progetti di Ricerca 2020

Investigation of higher-order structures of G-quadruplex multimers through extremely coarse-grained simulations**"Sapienza" Università di Roma****EUR 4.000**

12/2022 - Prot. N. RP12218162BCFD82

Principal Investigator: Cristiano De Michele

Progetti di Ricerca 2022

Taming structure, conformation and stability of multimeric G-quadruplex DNA (TAMeQUAD)**Ministero Università e Ricerca (MUR)****EUR 144.704**

Progetti di Ricerca di Rilevante Interesse Nazionale (PRIN) 2022

Project N. B53D23004500006

**National Principal Investigator: Cristiano De Michele**PART VII  
RESEARCH ACTIVITIES

## Keywords

Monte Carlo Simulations, Molecular Dynamics, Brownian Dynamics, Event-Driven Simulations, Coarse-Graining, Glasses, Supercooled Liquids, Gels, Colloids, Patchy Particles, Self-Assembly, Liquid Crystals, Cholesteric, Lyotropic, Polymers, Elastic Constants, numerical algorithms

Brief Description  
(cited numbers refer to the full list  
of publications reported in Part X)

Cristiano De Michele is a **theoretical and computational physicist** working in Condensed Matter Physics. In his work Cristiano develops novel theoretical approaches based on classical statistical mechanics and in-house codes (mostly in C and C++) for performing computer simulations. In the context of complex many-body systems such as glasses, gels, supercooled liquids, colloids and liquid crystals the main interests of his research activity are the development (i) of new theoretical approaches for calculating structural, thermodynamic and transport properties, (ii) of coarse-grained models and (iii) of novel algorithms for carrying out Monte Carlo, molecular dynamics (both event-driven and time-driven) and brownian simulations.

**Pisa: June 1997 - March 1998 (Master Degree)**

As final graduation project Cristiano has been working at the University of Pisa under the supervision of Prof. Dino Leporini on the development of a molecular dynamics code to study a model molecular glass former (namely rigid dumbbells) [1,2]. The aim of this project was to find for the first time clear evidence of a decoupling between jump dynamics and viscous flow - i.e. of the breakdown of the Stokes-Einstein (SE) and Debye-Stokes-Einstein (DSE) laws - in a molecular glass-former. Relaxation and transport properties of the model were extensively studied for both translational [1] and orientational [2] degrees of freedom through computer simulations providing unambiguous proof of the SE and DSE breakdown. Our study showed that SE and DSE expressions are verified in liquids only if the system is not supercooled.

**Naples-Rome: January 1999 - December 2003 (PhD)**

At University of Naples, under the supervision of Prof. Antonio Coniglio, Cristiano studied the dependence of the fragility of glass forming supercooled liquids on the softness of their interaction potential. At that time one of the main challenge in the physics of supercooled liquids and glasses was to understand the connection between the fragility and microscopic properties of the constituent particles. With this ambitious aim, Cristiano carried out molecular dynamics simulations of a simple glass-formers (binary mixture of soft spheres with tunable repulsion), showing unexpectedly that dynamic and thermodynamic fragility are both independent of the hard core repulsions between particles and that this independence can not be ascribed to a simple overall rescaling of the potential energy landscape [7].

**Rome: January 2004 - December 2007**

At University of Rome as a postdoctoral fellow Cristiano carried on with his studies on molecular and simple supercooled liquids. To grasp some understanding of the intriguing phenomenological result, which has been called "universal scaling", Cristiano developed, in collaboration with Prof. Dino Leporini group, a simple theory, which makes a strong connection between the structural relaxation time of glassy systems and the amplitude of the rattling oscillations of particles within the cage formed by their first neighbors [20]. Interestingly, the universal scaling makes no distinction between fragile and strong glasses and between molecular and simple glass-formers, thus providing a surprisingly unifying view to glassy systems. Afterwards, Cristiano attempted a first successful generalization of this universal scaling to colloidal gels as well [35], thus extending universal scaling to low concentration arrested states.

Concerning molecular glasses another open and challenging issue was the existence of a purely orientational glass. Hence, Cristiano further investigated the role of shape anisotropy in molecular glasses focusing on large particle elongations. Through a novel very efficient in-house event-driven code for simulating arbitrary hard convex bodies [30], Cristiano found for the first time evidence of a purely orientational glass transition in a system of uniaxial hard ellipsoids, confirming the theoretical predictions based on the Mode Coupling Theory [18].

Low concentration arrested states, also called gel states, were thought to be intimately connected to glassy states. In collaboration with Prof. Giuseppe Foffi, Cristiano started also working on the study of transport properties of colloidal gel systems. The possibility of having a gel state without any intervening phase separation in short-range attractive colloids generated huge debate in the soft matter community at that time. Cristiano developed a novel algorithm for carrying out brownian dynamics simulation of short-range attractive colloids interacting via a square-well potential [17]. Latter algorithm was employed to establish that scaling of dynamics in short-range attractive colloids is independent of microscopic dynamics [9], thus providing a first strong numerical evidence that disordered arrested states in short-range attractive colloids can be generated only as a result of a kinetically arrested phase separation [9,10]. To answer if it is possible to obtain a ("ideal") gel state along a reversible (equilibrium) path without any intervening phase separation, Cristiano started working on the quest for an "ideal gel state". Since a limited valence attractive interaction seemed a promising way to obtain such an "ideal gel", Cristiano developed an event-driven code for simulating hard spheres decorated with attractive ("patchy") spots and in a couple of papers, where primitive models of water [13] and silica [14] have been employed, evidence of an arresting mechanism at low concentration without any intervening phase separation was found for the first time.

**Rome-Lausanne-Pisa: January 2008 - September 2009**

Crowding (excluded volume) effects, which are closely related to structural (glassy) arrest, are expected to impact profoundly on the thermodynamics and kinetics of biological processes *in vivo*. Crowding effects on diffusion-limited reactions, which are commonly found in biochemical processes, such as antibody-antigen binding, enzyme catalysis, protein aggregation, and complexation in cells, had been examined only at low density of diffusing particles or for tracers diffusing in a medium of inert particles. Cristiano, while he was visiting scientist at EPFL in Lausanne, worked on the development of a coarse-grained model of diffusion-limited reactions in a crowded environment building on his past experience on colloidal systems. He performed brownian dynamics simulations using the algorithm developed by himself [17] and he proved the inadequacy of the state-of-the-art theory of diffusion-limited reactions, proposing a suitable generalization [33].

The algorithm developed by Cristiano for studying ideal gels was limited to patchy spheres, although shape anisotropy could have huge consequences on physical properties of patchy colloids. Cristiano generalized the event-driven code for simulating hard convex bodies making possible to arbitrarily decorate particles with attractive sites. This generalized code opened up the way to study transport properties of anisotropic patchy colloids offering a great flexibility in the design of the model to



simulate. In Ref. [23] a patchy particle model inspired by stepwise polymerization of an epoxy resin was introduced and studied by this novel event-driven code. In this paper we fully characterized the chemical gelation of this model according to existing theories for step polymerization. In this study we also developed several numerical tools for performing very efficiently the cluster analysis of the gel network, which proved to be very useful also lately [55]. In two successive publications we also connected irreversible to reversible aggregation in this system [27] and we provided an analytical description of the full aggregation kinetics [31]. Recently, we also developed and study through the event-driven code of Cristiano an autocatalytic patchy particle model, which provided, for the first time, a physical understanding of the reaction kinetics of epoxy resins [58].

#### **Rome: December 2009 - present**

Having acquired a broad experience in anisotropic patchy colloids, Cristiano's scientific interest was captured by patchy colloidal liquid crystals, where elongated conformation of their constituent particles plays a crucial role in their structural ordering. In particular, as non-tenure assistant professor at University of Rome, Cristiano focused his research activity on self-assembly-driven lyotropic liquid crystals, such as the ones obtained from the self-assembly of short DNA duplexes. While the isotropic-nematic transition in rigid and semi-flexible polymers had been investigated in detail, much less was known for the case a self-assembly-driven transition. The lack of an adequate theoretical description of these systems motivated Cristiano to develop a novel theoretical approach [38], whose predictions were in very good quantitative agreement with experimental results [39]. In addition, an accurate numerical assessment of the validity of this theory had been further provided by utilizing two simple models, i.e. bifunctional polymerizing hard cylinders [46] and bent-cylinders [48], in Monte Carlo simulations. Structural properties, such as radial distribution function and static structure factor, had been also calculated for some model systems finding a remarkable agreement between simulations results and theoretical predictions [43,50].

In concentrated solution of chiral particles, such as short DNA duplexes, G-quadruplexes, cellulose nanocrystals and many others, structural long-range ordering may manifest as a helical rotation of the alignment (nematic) axis. The connection between microscopic chirality of the constituent particles and macroscopic chiral ordering was far from being understood, since it was a challenge both for theory and computations. Cristiano was strongly motivated by the challenging nature of this scientific problem and he started working on the attempt to extend his previous theory of self-assembly-driven nematization to cholesteric lyotropic liquid crystals in collaboration with Prof. Alberta Ferrarini. Eventually, a successful theoretical framework was developed [53]. Theoretical predictions for the magnitude of the cholesteric pitch and its dependence upon both temperature and concentration were in good agreement with experiments, which had been carried out by Prof. Tommaso Bellini and Dott. Giuliano Zanchetta in Milano. Noticeably, our accurate theoretical treatment allowed us to afford for the first time a deep insight into the physical mechanisms underlying the formation of self-assembly-driven cholesteric liquid crystals out of short DNA duplexes. Our theoretical treatment has been extended to the calculation of all elastic constant [59] and theoretical predictions have been successfully compared to numerical and experimental results. Very recently, in collaboration with the group of Prof. R. Mezzenga at ETH, this theoretical treatment allowed us to gain a deep understanding of the physical mechanisms behind the formation of cholesteric phases of short amyloid fibrils [61].

The numerical study of chromonics and short DNA duplexes relies on efficient algorithms to simulate hard cylinders. Cristiano developed a novel and very efficient code for simulating hard cylinders [57], which required also the development of a novel algorithm for solving quartic equations. The corresponding paper has been published in ACM Transactions on Mathematical Software.

Among all LC phases observed in self-assembly-driven liquid crystals based on DNA, the smectic one was elusive so far. Building on DNA versatility in creating novel constructs and our former theoretical understanding of self-assembly-driven liquid crystal phases we designed three DNA sequences which self-assemble at room temperature into a nanoparticle about 50 nm long comprising of two double-stranded DNA duplexes linked together by a DNA filament 13 nm long. This nanoparticle resembles a nunchaku which is the traditional weapon of several martial arts, such as kung-fu and ju-jitsu, their size being 30 millions times smaller though. Recently, we have provided unambiguous and clear evidence through experiments and numerical simulations that a water suspension of these synthetic DNA nanonunchakus form smectic phases [56]. In a more recent follow-up of this work we provided experimental and numerical evidence of smectic phases obtained from patchy DNA rods [66].

The scientific interest of Cristiano for crowding effects in biological systems was still rather alive and he found a fertile ground for his ideas on the subject in the problem of antibody-antigen binding. Antibodies play a prominent role in the human immune systems, because they are capable of forming complexes with pathological intruders, not matter their size and shape, thus eliciting an immune



response. A fundamental question concerning this biophysical process is: what makes antibodies so effective? To answer this question of paramount importance for biophysics Cristiano developed an extremely "coarse-grained" model of IgG antibodies to better understand their interaction with simple antigens. A careful combined analysis of numerical data from computer simulations and experimental results available in literatures allowed him to develop a very accurate theoretical paradigm, beyond existing frameworks, to interpret experimental profiles of antibodies binding to multivalent surfaces of different sorts and to grasp some understanding of the surprising binding ability of antibodies [54].

Shape anisotropy of colloidal particles may have a role also in the formation of gel as a result of a kinetically arrested phase separation. Prof. Peter Schurtenberger and co-workers after having evidenced in recent novel experiments an unusual dynamics in solution of attractive globular proteins asked Cristiano to develop a suitable extremely coarse-grained model of the globular protein to carry out computer simulations. Numerical results obtained from computer simulations performed by Cristiano contributed to shed light on the experimental observations. Indeed, since static properties of the globular protein were in quantitative agreement with predictions for binary liquid mixtures, the richer and more complex behavior of dynamics could be ascribed to a competition between critical slowing down and dynamical arrest [52]. In collaboration with Prof. Schurtenberger, Cristiano recently investigated numerically through Monte Carlo simulations the role played by particle shape in magnetic-field-assisted assembly of prolate colloids, where a subtle deviation from the ideal ellipsoidal shape of particles dictates the formation of an unusual sequence of field-induced structures, which include an unexpected oblate smectic phase [67].

Since 2018, in collaboration with Prof. Lara Benfatto of University of Rome "Sapienza", in the last year Cristiano attempted to further develop the known analogy between soft matter systems and superconductor. In thin films of type-II semiconductors 2D Abrikosov vortices emerge by applying a suitable transverse magnetic field at low temperatures. These vortices effectively behave like colloidal particles and they can exhibit the rich phase diagram predicted for these systems with a solid, hexatic and liquid phases. He investigated numerically the static and dynamic properties of 2D Abrikosov vortices by means of computer simulations where the evolution of each single vortex was tracked to extract static and dynamical properties of the system. Moreover, concerning the dynamics it was found evidence of a fragile to strong transition on changing the strength of the magnetic field, i.e. the quenched disorder of the system [69]. Another ongoing collaboration within the Department of Physics of "Sapienza" is with Prof. Livia Bove with whom Cristiano is studying both numerically and experimentally hydrogen hydrates, reporting for the first time evidence of their most H<sub>2</sub>-dense phase (C3 phase) [72].

More recently, in collaboration with Prof. Alessandro Paciaroni (University of Perugia), Dott. Lucia Comez (CNR-IOM Perugia) and Prof. Bruno Pagano (Department of Pharmacy, University of Naples Federico II) Cristiano is investigating non-canonical structures, called G-quadruplexes, which form in the telomeric part of humane genome [71]. These structures may multimerize and give rise to higher-order structures where the different G4 units may interact with each other. In recent years multimeric G4s have been shown to be key in protecting or disrupting the pathogenic cascade of various diseases, such as cancer and neuropathies. However, the large-scale structure, conformation and stability properties of G4 multimers are still a matter of heated debate. The aim of this collaboration is to provide a clear picture of those properties for the paradigmatic case of G4 multimers that form from extended single-stranded human telomere sequences. He is also studying G4 multimers in presence of crowders agents and of benchmark ligands (i.e. potential anticancer drugs).

Finally, over recent years Cristiano fruitfully collaborated with Prof. Giovanni Ciccotti, with whom he tackled fundamental issues in molecular dynamics algorithm. A first achievement of this collaboration has been a novel measure-preserving and reversible algorithm for carrying out isothermal-isobaric molecular dynamisc simulations of molecular systems with constraints [74].

#### List of Research Activities

- Development of novel brownian dynamics algorithms for stochastic event-driven simulations
- Development of novel algorithms for event-driven molecular dynamics simulation of generic hard rigid bodies decorated with localized stepwise ("patchy") interactions
- Optimization of numerical methods employed in event-driven simulations, like multidimensional root finding and multidimensional minimization of functions
- Multi-scale modeling of biophysical and colloidal systems combining atomistic models, mesoscale (coarse-grained) models and continuum models
- Design of "patchy" models for studying chemical gelation and irreversible aggregation of model systems
- Coarse-grained models for biophysical and colloidal systems
- Study of static and dynamical properties of simple and molecular supercooled liquids: structure, rheology, diffusivity and relaxation

- Study of the glass transition in simple model systems with potential energy landscape approach
- Investigation of short-range attractive colloids through computer simulations: gel transition, arrested phase separation, aging and viscoelasticity
- Static and dynamic properties of hard ellipsoids: molecular correlation functions and isotropic-nematic (liquid crystal) transition
- Role of reduced valence and directionality in colloidal systems
- Universal scaling for gels, polymers and glassy systems as a unifying view to complex systems
- Self-assembly of DNA duplexes into polymers chains: theory and simulations
- Molecular theory of elasticity for self-assembly-driven cholesteric liquid crystals
- Novel numerical techniques for carrying out molecular dynamics simulations
- Modeling and numerical study of telomeric multimeric G4s.

Scientific Interests

Computational Physics

- Molecular dynamics simulations
- Event-driven simulations
- Monte Carlo simulations
- Stochastic dynamics
- High-performance computing

Soft and Condensed Matter

- Glass transition
- Gelation
- Theory of simple and molecular liquids
- Colloidal systems
- Reversible Polymers
- Self-Assembly in Colloidal Systems
- Self-assembly-driven Lyotropic Liquid Crystals

PART VIII  
SUMMARY OF  
SCIENTIFIC ACHIEVEMENTS

Number of Publications 75 (Total)  
72 (Scopus)

Number of Publications 47 (Total)  
(over last 15 years) 46 (Scopus)

Total Number of Citations 2452 (Scopus)  
3176 (Google Scholar)

Total Number of Citations 1054 (Scopus)  
(over last 15 years)

H-index 32 (Scopus)  
34 (Google Scholar)

H-index (over last 15 years) 20 (Scopus)

Total Impact Factor 388.8

Total Impact Factor 280.2  
(over last 15 years)

Average Citations per publication 42.6 (Google scholar)  
35 (Scopus)

Average Citations per publication 22.9 (Scopus)  
(over last 15 years)

Average Impact Factor per publication 5.4

Average Impact Factor per publication 6.0  
(over last 15 years)

Normalized H-index 1.62 (Google scholar)  
(by academic seniority) 1.52 (Scopus)

Normalized H-index 1.33 (Scopus)  
(over last 15 years)

Research ID C-2345-2015

ORCID [orcid.org/0000-0002-8367-0610](https://orcid.org/0000-0002-8367-0610)

## PART IX FURTHER INFORMATION

### Computer Science Skills

#### ▪ Operating Systems

Linux, BSD, Microsoft Windows e Mac OSX

#### ▪ Software Development

##### **Linux**

From 2003 to 1<sup>st</sup> March 2008 (closing date of the project) I was an OpenMosix developer (home page: <http://www.openmosix.org>, project leader: [Dr. Moshe Bar](#)). OpenMosix was an open source project hosted by [Sourceforge](#) providing a linux kernel patch and some user tools for realizing Single System Image (SSI) clusters. I contributed to this project with several extensions both on kernel and user interface side.

##### **Computer Simulations**

During my research activity I developed many codes, written in C and C++, to carry out serial and parallel simulations of many-body systems, to analyse data and visualize simulated particles.

#### ▪ High-performance computing

I use SSI clusters based on Mosix which I contribute to administer as well.

#### ▪ Programming Languages

C/C++, Assembly x86, Fortran 77/90, Pascal, Visual Basic, SQL e Python.

#### ▪ Office Tools

LaTeX, TeX, OpenOffice, Microsoft Office, Mathematica.

#### ▪ Simulations Packages

GROMACS

#### ▪ Libraries

MPI, System V IPC, openMP, openGL e Gtk+/Gnome.

#### ▪ Development Tools

git, cvs, subversion, make

### Full List of Publications

1. *Viscous flow and jump dynamics in molecular supercooled liquids: I Translations*  
**C. De Michele** and D. Leporini  
Physical Review E **63**, 036701 (2001)
2. *Viscous flow and jump dynamics in molecular supercooled liquids: II Rotations*  
**C. De Michele** and D. Leporini  
Physical Review E **63**, 036702 (2001)

3. *Equilibration times in numerical simulation of structural glasses: Comparing parallel tempering and conventional molecular dynamics*  
**C. De Michele** and F. Sciortino  
Physical Review E **65**, 051202 (2002)
4. *Molecular dynamics studies of biatomic supercooled liquids: intermittency, stick-slip transition and the breakdown of the Stokes-Einstein laws" in "Scaling and Disordered Systems*  
**C. De Michele** and D. Leporini  
Fractals - Complex Geometry Patterns and Scaling in Nature and Society **11**, 139-147 (2003)
5. *Numerical evaluation of the statistical properties of a potential energy landscape*  
E. La Nave, F. Sciortino, P. Tartaglia, **C. De Michele** and S. Mossa  
Journal of Physics: Condensed Matter **15**, S1085-S1094 (2003)
6. *Landscape and fragilities*  
G. Ruocco, F. Sciortino, F. Zamponi, **C. De Michele** and T. Scopigno  
Journal of Chemical Physics **120**, 10666 – 10680 (2004)
7. *Scaling in soft spheres: fragility invariance on the repulsive potential softness*  
**C. De Michele**, F. Sciortino and A. Coniglio  
Journal of Physics: Condensed Matter **16**, L489-L494 (2004)
8. *Saddles and softness in simple model liquids,*  
L. Angelani, **C. De Michele**, G. Ruocco and F. Sciortino  
J. Chem. Phys. **121**, 7533-7534 (2004)
9. *Scaling of dynamics with the range of interaction in short-range attractive colloids*  
G. Foffi, **C. De Michele**, F. Sciortino and P. Tartaglia  
Physical Review Letters **94**, 078301 (2005)
10. *Arrested phase separation in a short-ranged attractive colloidal system: a numerical study*  
G. Foffi, **C. De Michele**, F. Sciortino and P. Tartaglia  
Journal of Chemical Physics **122**, 224903 (2005)  
[ see also comment by S. Sastry: Nature **441**, 671 (2006) ]
11. *Routes to Colloidal Gel Formation*  
F. Sciortino, S. Buldyrev, **C. De Michele**, G. Foffi, N. Ghofraniha, E. La Nave, A. Moreno, S. Mossa, I. Saika-Voivod, P. Tartaglia and E. Zaccarelli  
Computer Physics Communications **169**, 166-171 (2005)
12. *Molecular Correlation Functions for Uniaxial Ellipsoids in the Isotropic State*  
**C. De Michele**, A. Scala, R. Schilling and F. Sciortino  
Journal of Chemical Physics **124**, 104509 (2006)
13. *Dynamics in the presence of attractive patchy interactions*  
**C. De Michele**, S. Gabrielli, F. Sciortino and P. Tartaglia  
Journal of Physical Chemistry B **110**, 8064-8079 (2006)
14. *Slow dynamics in a primitive tetrahedral network model*  
**C. De Michele**, P. Tartaglia and F. Sciortino  
Journal of Chemical Physics **125**, 204710 (2006)
15. *Gel and Glass transitions in Short-Range Attractive Colloidal Systems*  
G. Foffi, N. Dorsaz and **C. De Michele**  
in "Food Colloids: Self-Assembly and Material Science"  
Edited by E. Dickinson and M. E. Leser, RSC Publishing Issue: 302, 327-342 (2007)
16. *Aging in a Laponite colloidal suspension: A Brownian dynamics simulation study*  
S. Mossa, **C. De Michele** and F. Sciortino  
Journal of Chemical Physics **126**, 014905 (2007)
17. *Event-Driven Brownian Dynamics for Hard Spheres*  
Th. Voigtmann, A. Scala and **C. De Michele**  
Journal of Chemical Physics **126**, 134109 (2007)

18. *Dynamics of uniaxial hard ellipsoids*  
**C. De Michele**, F. Sciortino and R. Schilling  
Physical Review Letters **98**, 265702 (2007)
19. *Viscoelasticity and Stokes-Einstein relation in repulsive and attractive colloidal glasses*  
A. Puertas, **C. De Michele**, F. Sciortino, P. Tartaglia and E. Zaccarelli  
Journal of Chemical Physics **127**, 144906 (2007)
20. *Universal scaling between structural relaxation and vibrational dynamics in glass-forming liquids and polymers*  
L. Larini, A. Ottochian, **C. De Michele** and D. Leporini  
Nature Physics **4**, 42-45 (2008)
21. *Event-driven Simulation of the Dynamics of Hard Ellipsoids*  
**C. De Michele**, R. Schilling and F. Sciortino  
AIP Conference Proceedings of IWCS2007 (Sendai, Japan) **982**, 148-153 (2008)
22. *Growth of equilibrium polymers under non-equilibrium conditions*  
F. Sciortino, J. Douglas and **C. De Michele**  
Journal of Physics: Condensed Matter **20**, 155101 (2008)
23. *A molecular dynamics study of chemical gelation in a patchy particle model*  
S. Corezzi, **C. De Michele**, E. Zaccarelli, D. Fioretto and F. Sciortino  
Soft Matter **4**, 1173-1177 (2008)
24. *The influence of bond-rigidity and cluster diffusion on the self-diffusion of hard-spheres with square-well interaction*  
S. Babu, J. C. Gimel, T. Nicolai and **C. De Michele**  
Journal of Chemical Physics **128**, 204504 (2008)
25. *Simulation of the Dynamics of Hard Ellipsoids*  
**C. De Michele**, R. Schilling and F. Sciortino  
Proceedings of "XI International Workshop on Complex Systems" (Andalo, Italy)  
Editors A. Fontana, P. Verrocchio and G. Viliari (2008)
26. *Non-gaussian effects in the cage dynamics of polymers*  
A. Ottochian, **C. De Michele** and D. Leporini  
Proceedings of "XI International Workshop on Complex Systems" (Andalo, Italy)  
Editors A. Fontana, P. Verrocchio and G. Viliari  
Philosophical Magazine **88**, 4057-4062 (2008)
27. *Connecting Irreversible to Reversible Aggregation: Time and Temperature*  
S. Corezzi, **C. De Michele**, E. Zaccarelli, P. Tartaglia and F. Sciortino  
Journal of Physical Chemistry B **113**, 1233-1236 (2009)
28. *A parameter-free description of the kinetics of formation of loop-less branched structures and gels*  
F. Sciortino, **C. De Michele**, S. Corezzi, J. Russo, E. Zaccarelli and P. Tartaglia  
Soft Matter **5**, 2571-2575 (2009)
29. *Universal divergenceless scaling between structural relaxation and caged dynamics in glass-forming systems*  
A. Ottochian, **C. De Michele** and D. Leporini  
Journal of Chemical Physics **131**, 224517 (2009)
30. *Simulating Hard Rigid Bodies*  
**C. De Michele**  
Journal of Computational Physics **229**, 3276-3294 (2010)
31. *Modeling the Crossover between Chemically and Diffusion-Controlled Irreversible Aggregation in a Small-Functionality Gel-Forming System*  
S. Corezzi, D. Fioretto, **C. De Michele**, E. Zaccarelli and F. Sciortino  
Journal of Physical Chemistry B **114**, 3769-3775 (2010)
32. *Inertial effect in diffusion-limited reactions*  
N. Dorsaz, **C. De Michele**, F. Piazza and G. Foffi

- Journal of Physics: Condensed Matter **22**, 104116 (2010)
33. *Diffusion Limited Reactions in Crowded Environments*  
N. Dorsaz, **C. De Michele**, F. Piazza, P. Del Los Rios and G. Foffi  
Physical Review Letters **105**, 120601 (2010)  
[ see also related viewpoint: "Speeding up in a crowd", H.-X. Zhou, Physics **3**, 77 (2010) ]
34. *Crowding, Intermolecular Interactions and Shear Flow Effects in the Diffusion Model of Chemical Reactions*  
A. Zaccone., N. Dorsaz, F. Piazza, **C. De Michele**, M. Morbidelli and G. Foffi  
Journal of Physical Chemistry B **115**, 7383-7396 (2011)
35. *Scaling between Structural relaxation and particle caging in a model colloidal gel*  
**C. De Michele**, E. Del Gado and D. Leporini  
Soft Matter **7**, 4025-4031 (2011)
36. *Optimizing Event-Driven Simulations*  
**C. De Michele**  
Computer Physics Communications **182**, 1846-1850 (2011)
37. *Monte Carlo and event-driven dynamics of Brownian particles with orientational degrees of freedom*  
F. Romano, **C. De Michele**, D. Marenduzzo, and E. Sanz  
Journal of Chemical Physics **135**, 124106 (2011)
38. *Self-assembly of bi-functional patchy particles with anisotropic shape into polymers chains: theory, simulations and experiments*  
**C. De Michele**, T. Bellini and F. Sciortino  
Macromolecules **45**, 1090-1106 (2012)
39. *Self-assembly of short DNA duplexes: from a coarse-grained model to experiments through a theoretical link*  
**C. De Michele**, L. Rovigatti, T. Bellini and F. Sciortino  
Soft Matter **8**, 8388 – 8398 (2012)
40. *Disordered Systems - Predicting the Ultra-Slow Processes by Picosecond Dynamics*  
A. Ottochian, **C. De Michele**, F. Puosi and D. Leporini  
Il Nuovo Saggiatore **28**, 5-10 (2012)
41. *Comment on "Generalized localization model of relaxation in glass-forming liquids*  
A. Ottochian, F. Puosi, **C. De Michele** and D. Leporini  
Soft Matter **9**, 7890-7891 (2013)
42. *Irreversible bimolecular reactions with inertia: from the trapping to the target setting at finite densities*  
F. Piazza, G. Foffi and **C. De Michele**  
Journal of Physics: Condensed Matter **25**, 245101 (2013)
43. *How to calculate structure factors of self-assembling anisotropic particles*  
S. Kantorovich, E. Pyanzina, **C. De Michele** and F. Sciortino  
Soft Matter **9**, 4412-4427 (2013)
44. *Scaling between relaxation, transport and caged dynamics in a binary mixture on a per-component basis*  
F. Puosi, **C. De Michele** and D. Leporini  
Journal of Chemical Physics **138**, 12A532 (2013)
45. *Diffusion-limited reactions in crowded environments: a local density approximation*  
F. Piazza, N. Dorsaz, **C. De Michele**, P. des Los Rios and G. Foffi  
Journal of Physics: Condensed Matter **25**, 375104 (2013)
46. *Self-Assembly-Driven Nematization*  
K. T. Nguyen, F. Sciortino and **C. De Michele**  
Langmuir **30**, 4814-4819 (2014)



47. *Self-Assembly of hard helices: a rich and unconventional polymorphism*  
H. Bindu Kolli, E. Frezza, G. Cinacchi, A. Ferrarini, A. Giacometti, T. S. Hudson,  
**C. De Michele** and F. Sciortino  
Soft Matter **10**, 8171-8187 (2014)
48. *Self-Assembly of mesogenic bent-core DNA nanoduplexes*  
K. T. Nguyen, A. Battisti, D. Ancora, F. Sciortino and **C. De Michele**  
Soft Matter **11**, 2934-2944 (2015)
49. *Modelling the rheology of anisotropic particles adsorbed on a two-dimensional fluid interface*  
A. M. Luo, L. M. C. Sagis, H. C. Ottinger, **C. De Michele** and O. Ilg  
Soft Matter **11**, 4383-4395 (2015)
50. *Nematic phase characterisation of the self-assembling sphere-cylinders based on the theoretically calculated RDFs*  
E. S. Pyanzina, **C. De Michele** and S. S. Kantorovich  
The European Physical Journal E **38**, 81 (2015)
51. *Non-universal Voronoi cell shapes in amorphous ellipsoid packs*  
F. M. Schaller, S. C. Kapfer, J. E. Jilton, P. W. Clearly, K. Mecke, **C. De Michele**, T. Schilling,  
M. Saadatfar, M. Schröter, G. W. Delaney, G. E. Schröder-Turk  
Europhysics Letters **111**, 24002 (2015)
52. *Unusual Dynamics of Concentration Fluctuations in Solutions of Weakly Attractive Globular Proteins*  
S. Bucciarelli, L. Casal-Dujat, **C. De Michele**, F. Sciortino, J. Dhont, J. Bergenholtz,  
B. Farago, P. Schurtenberger e A. Stradner  
Journal of Physical Chemistry Letters **6**, 4470-4474 (2015)
53. *Hierarchical Propagation of Chirality through Reversible Polymerization: The Cholesteric Phase of DNA Oligomers*  
**C. De Michele**, G. Zanchetta, T. Bellini, E. Frezza and A. Ferrarini  
ACS MacroLetters **5**, 208-212 (2016)
54. *Simulation and Theory of Antibody Binding to Crowded Antigen-Covered Surfaces*  
**C. De Michele**, P. De Los Rios, G. Foffi and F. Piazza  
PLOS Computational Biology **12** (3): e1004752, doi:10.1371/journal.pcbi.1004752 (2016)
55. *Anomalous dynamics of intruders in a crowded environment of mobile obstacles*  
T. Sentjabrskaja, E. Zaccarelli, **C. De Michele**, F. Sciortino, P. Tartaglia, T. Voigtmann,  
S. U. Egelhaaf and M. Laurati  
Nature Communications **7**:11133, doi: 10.1038/ncomms11133 (2016)
56. *Smectic phase in suspensions of gapped DNA duplexes*  
M. Salamonczyk, J. Zhang, G. Portale, C. Zhu, E. Kentzinger, J. T. Gleeson, A. Jakli,  
**C. De Michele**, J. K. G. Dhont, S. Sprunt and E. Stiakakis  
Nature Communications **7**, 13358 (2016)
57. *Speeding up Monte Carlo Simulation of Patchy Hard Cylinders*  
A. Orellana, E. Romani and C. De Michele  
invited contribution to the European Journal E Special Issue  
"Advances in Computational Methods for Soft Matter Systems"  
Eur. Phys. J E **41**, 51 (2018); doi: 10.1140/epje/i2018-11657-0
58. *Exploiting Limited Valence 'Patchy' Particles to Understand Autocatalytic Kinetics*  
S. Corezzi, F. Sciortino and **C. De Michele**  
Nature Communications **9**, 2647 (2018); doi: 10.1038/s41467-018-04977-0
59. *Elastic Constants of Chromonic Liquid Crystals*  
E. Romani, A. Ferrarini and **C. De Michele**  
Macromolecules **51**, 5409-5419 (2018); doi: 10.1021/acs.macromol.8b00900
60. *Nematic liquid crystals of bifunctional patchy spheres*  
K. T. Nguyen and **C. De Michele**  
Eur. Phys. J. E **41**, 141 (2018) – doi:10.1140/epje/i2018-11750-4



61. *Amyloid Fibrils Length Controls Shape and Structure of Nematic and Cholesteric Tactoids*  
M. Bagnani M., G. Nystrom, **C. De Michele** and R. Mezzenga  
ACS Nano **13**, 591-600 (2019) – doi: 10.1021/acsnano.8b07557
62. *Free energy of conformational isomers: The case of gapped DNA duplexes*  
A. G. Orellana and **C. De Michele**  
Eur. Phys. J. E **42**, 71 (2019)
63. *Theory of self-assembly-driven nematic liquid crystals revised*  
**C. De Michele**  
Liquid Crystals, doi: 10.1080/02678292.2019.1645366 (2019)
64. *Boosting Efficiency in Solving Quartic Equation with no Compromise on Accuracy*  
A. Orellana and **C. De Michele**,  
ACM Transactions on Mathematical Software Vol. **46**, No. 2, Article 20 (2020).
65. *Elastic constants of biological filamentous colloids: estimation and implications on nematic and cholesteric tactoid morphologies*  
M. Bagnani, P. Azzari, **C. De Michele**, M. Arcari and R. Mezzenga  
Soft Matter **17**, 2158-2169 (2021)
66. *Self-Assembly of All-DNA Rods with Controlled Patchiness*  
K. Gvozden, S. N. Ratajczak, A. G. Orellana, E. Kentzinger, U. Rücker, J. K. G. Dhont, **C. De Michele** and E. Stiakakis  
Small **21**04510, doi: 10.1002/smll.202104510 (2021)
67. *Shape Matters in Magnetic-Field-Assisted Assembly of Prolate Colloids*  
A. Pal, C. A. De Filippo, T. Ito, Md. A. Kamal, A. V. Petukhov, **C. De Michele**, and P. Schurtenberger  
ACS Nano **16**, 2558-2568 (2022)
68. *Remark on Algorithm 1010: Boosting Efficiency in Solving Quartic Equations with No Compromise in Accuracy*  
C. De Michele  
ACM Transactions on Mathematical Software, Vol. **48** No. 4 (2022)
69. *Transport signatures of fragile glass dynamics in the melting of the two-dimensional vortex lattice*  
I. Maccari, Bal K. Pokharel, J. Terzic, Surajit Dutta, J. Jesudasan, Pratap Raychaudhuri, J. Lorenzana, **C. De Michele**, C. Castellani, L. Benfatto, Dragana Popovic  
Phys. Rev. B **107**, 014509 (2023)
70. *On the role of polydispersity on the phase diagram of colloidal rod*  
C. A. De Filippo, S. Del Galdo, P. Corsi, C. De Michele and B. Capone  
Soft Matter, **19** 1732-1738 (2023)
71. *Stacking Interactions and Flexibility of Human Telomeric Multimers*  
B. P. Rosi, V. Libera, L. Bertini, A. Orecchini, S. Corezzi, G. Schirò, P. Pernot, R. Biehl, C. Petrillo, L. Comez, C. De Michele and A. Paciaroni  
J. Am. Chem. Soc. **145**, 29, 16166–16175 (2023)
72. *Observation of the most H<sub>2</sub>-dense filled ice under high pressure*  
U. Ranieri, S. Di Cataldo, M. Rescigno, L. Monacelli, R. Gaal, M. Santoro, L. Andriambariarijaona, P. Parisiadis, C. De Michele and L. E. Bove  
PNAS, **120** (52) e231266512 (2023)
73. *Remark on Algorithm 1010: Boosting Efficiency in Solving Quartic Equations with No Compromise in Accuracy*  
C. De Michele  
ACM Trans. Math. Softw., <http://dx.doi.org/10.1145/3674833> (2024)
74. *A correct, reversible Trotter splitting for the evolution operator in molecular dynamics simulations of molecular systems with constraints*  
C. De Michele and G. Ciccotti  
Mol. Phys. DOI: 10.1080/00268976.2024.2364834 (2024)

Selected List of N. 16  
Publications

1. *Stacking Interactions and Flexibility of Human Telomeric Multimers*  
B. P. Rosi, V. Libera, L. Bertini, A. Orecchini, S. Corezzi, G. Schirò, P. Pernot, R. Biehl, C. Petrillo, L. Comez, C. De Michele and A. Paciaroni  
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PNAS, **120** (52) e231266512 (2023)
3. *Shape Matters in Magnetic-Field-Assisted Assembly of Prolate Colloids*  
A. Pal, C. A. De Filippo, T. Ito, Md. A. Kamal, A. V. Petukhov, **C. De Michele**, and P. Schurtenberger  
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4. *Self-Assembly of All-DNA Rods with Controlled Patchiness*  
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Small **21**04510, doi: 10.1002/smll.202104510 (2021)
5. *Amyloid Fibrils Length Controls Shape and Structure of Nematic and Cholesteric Tactoids*  
M. Bagnani M., G. Nystrom, **C. De Michele** and R. Mezzenga  
ACS Nano **13**, 591-600 (2019) – doi: 10.1021/acsnano.8b07557
6. *Speeding up Monte Carlo Simulation of Patchy Hard Cylinders*  
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7. *Exploiting Limited Valence 'Patchy' Particles to Understand Autocatalytic Kinetics*  
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8. *Smectic phase in suspensions of gapped DNA duplexes*  
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9. *Hierarchical Propagation of Chirality through Reversible Polymerization: The Cholesteric Phase of DNA Oligomers*  
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11. *Unusual Dynamics of Concentration Fluctuations in Solutions of Weakly Attractive Globular Proteins*  
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12. *Elastic Constants of Chromonic Liquid Crystals*  
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13. *Simulation and Theory of Antibody Binding to Crowded Antigen-Covered Surfaces*  
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PLOS Computational Biology **12** (3): e1004752, doi:10.1371/journal.pcbi.1004752 (2016)
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16. *A correct, reversible Trotter splitting for the evolution operator in molecular dynamics simulations of molecular systems with constraints*  
C. De Michele and G. Ciccotti  
Mol. Phys. DOI: 10.1080/00268976.2024.2364834 (2024)

## International Conferences

**34** oral contributions to international conferences, including **11 invited talks**, as detailed below:

**15° National Conference - SICL**

Sirolo, Ancona, 26-28 May 2024 (**invited**)

**Frontiers in Water Biophysics**

Erice, Italia, 19-24 May 2023 (**invited**)

**14° National Conference - SICL**

Padova, 22-23 September 2022 (**invited**)

**Frontiers in Water Biophysics**

Erice, Italia, 21-26 July 2019 (**invited**)

**International Liquid Crystal Conference 2018 (ILCC2018)**

Kyoto, Giappone 22-27 Luglio 2018 (**invited**)

[ 747 participants, 52 invited talks out of 179 oral presentations ]

**Nanoinnovation 2018**

Roma, Italia, 11-14 Settembre 2018 (**invited**)

**9<sup>th</sup> Italian-Japanese Workshop on Liquid Crystals**

Pavia, Italia, 17-20 Settembre 2018 (**invited**)

**Italian Soft Days 2018**

Padova, Italia, 13-14 Settembre 2018

**DIRECTED STRUCTURE AT THE MESO-SCALE (DISTRUC)**

Heraklion, Creta 1-2 July 2017 (**invited**)

**TWISTED 2017**

Luxembourg, Luxembourg, 10-12 May 2017

**ECIS 2016**

Rome, Italy, 4 September - 9 September 2016

**European Conference on Liquid Crystals (ECLC2015)**

Manchester, UK, 7 September - 11 September 2015

**IACIS 2015**

Mainz, Germany, 24 - 29 May, 2015

**International Liquid Crystal Conference 2014 (ILCC2014)**

Dublin, Ireland, 29 June - 4 July 2014

**CECAM Workshop “DNA-based self-assembly: theory, simulations and experiments”**  
Vienna, Austria, 2 - 5 December 2013

**Le Studium Conference “Macromolecular Crowding Effects in Cell Biology: models and experiments”**  
Orleans, France, 24 - 25 October 2013 (invited)

**Conference “Programmable Self-Assembly of Matter”**  
New York, USA, 30 July - 2 June 2013

**CECAM Workshop “Design of Self-Assembling Materials”**  
Vienna, Austria, 4 - 7 September 2012 (invited)

**International Liquid Crystal Conference 2012 (ILCC2012)**  
Mainz, Germany, 19 - 24 August 2012

**XXIII Sitges Conference on Statistical Mechanics**  
Sitges, Barcelona, Spain, 4 - 8 June 2012

**Juelich Soft Matter Days (JSMD2011)**  
Bonn, Germany, 15 - 18 November 2011

**Liquid Matter Conference (LMC2011)**  
Vienna, Austria, 6 - 10 September 2011

**International Soft Matter Conference (ISMC2010)**  
Granada, Spain, 5 - 8 July 2010

**Conference on Computational Physics 2010 (CCP2010)**  
Trondheim, Norway, 22 - 26 June 2010

**CECAM Workshop “New Trends in Simulating Colloids: from Models to Applications”**  
EPFL Lausanne, Switzerland, 15 - 18 July 2009 (invited)

**XI International Workshop on Complex Systems**  
Andalo, Trento, Italy, 17 - 20 March 2008

**5<sup>th</sup> Workshop on Complex Systems (IWCS2007)**  
Sendai, Japan, 25 - 28 September 2007

**81<sup>st</sup> Colloid and Surface Symposium**  
Newark, Delaware, USA, 24 - 27 June 2007

**CECAM Workshop “Simulations of Hard Bodies”**  
Lyon, France, 16-19 April 2007

**Meeting on “Computer Simulations of Attractive Colloidal Particles”**  
organizzato dal Marie Curie Research and Training Network “Dynamical Arrested State of Soft Matter and Colloids”  
University of Le Mans, Le Mans, France, 19 - 12 November 2005

**Unifying Concepts in Granular Media and Glasses**  
Capri, Naples, Italy 19 - 20 May 2005

**Winter Discussion Workshop on Dynamical Arrest of Soft Matter and Colloids**  
Bad Gastein, Austria, 22 - 26 January 2005

**INFMEETING 2004**  
Genova, Italy, 8 - 10 June 2004

**Workshop on glass and complex systems**  
Capri, Naples, Italy, 14 - 16 June 2001

## Conference Organization

- **Co-organization of CECAM workshop:** *Exploring bio-inspired systems: a synergy between multiscale experimental and computational approaches*, Vienna, Austria from 4 to 7 September 2024.
- **Co-organization with Prof. Roberto Cerbino and Dr. Elisa Frezza of CECAM workshop:** *DNA-based self-assembly: theory, simulations and experiments*, Vienna, Austria from 2 to 5 December 2013.
- **Co-organization with Dr. Antonio Scala of CECAM workshop:** *Simulations of Hard Bodies*, CECAM-Lyon, France from 16 to 19 April 2007

## Invited Seminars

- |          |   |
|----------|---|
| 30/07/18 | Institute of Industrial Science, Department of Fundamental Engineering<br>The University of Tokyo, Tokyo, Giappone, title: " <i>Self-Assembly-Driven Colloidal Liquid Crystals</i> "<br>Invited by <b>Prof. H. Tanaka</b>   |
| 22/06/16 | Juelich Forschungszentrum, Juelich, Germany, title: " <i>Hierarchical propagation of chirality through reversible polymerization: the cholesteric phase of DNA oligomers</i> "<br>Invited by <b>Prof. J. K. G. Dhont</b>  |
| 02/06/16 | Loire Valley <b>Institute for Advanced Studies, Orleans</b> , France, title: " <i>Coarse-grained Modeling of Colloidal Suspensions</i> "<br>( <a href="http://www.lestudium-ias.com/event/coarse-grained-modeling-colloidal-suspensions">http://www.lestudium-ias.com/event/coarse-grained-modeling-colloidal-suspensions</a> ) |
| 09/01/16 | Department of Physics - <b>University of Paris Sud</b> , talk title: " <i>Hierarchical propagation of chirality through reversible polymerization: the cholesteric phase of DNA oligomers</i> "<br>Invited by <b>Prof. G. Foffi</b>   |
| 14/10/15 | Department of Chemistry, <b>University of Cambridge</b> , UK<br><i>Hierarchical propagation of chirality through reversible polymerization: the cholesteric phase of DNA oligomers</i><br>Invited by <b>Prof.ssa E. Eiser</b>   |
| 01/12/06 | <b>École Polytechnique Fédérale de Lausanne (EPFL)</b> a Lausanne, Switzerland<br><i>Hard ellipsoids: structure and theory</i><br>Invited by <b>Prof. Giuseppe Foffi</b>  |
| 25/04/06 | Department of Physics, <b>University of Konstanz</b> , Germany<br><i>Hard ellipsoids: structure and theory</i><br>Invited by <b>Prof. Matthias Fuchs</b>  |

## Commission of Trust

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|--------------|--|
| 2003-present | <b>Reviewer for Scientific Journals, such as:</b> Physical Review Letters, Soft Matter, Journal of Chemical Physics, Physical Chemistry Chemical Physics, Journal of Physical Chemistry, Physical Review E, Journal of Non-crystalline Solids, Computational Physics Communications, Journal of Computational Physics, The European Journal E. |
| 2014-present | Book Proposal Reviewer for John Wiley & Sons Limited   |
| 2014-present | Evaluator for Scientific Agencies: Deutsche Forschungsgemeinschaft (German Research Foundation) and ACS Petroleum Research Fund (USA)  |

## Institutional Responsibilities

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|--------------|--|
| 2014-2017    | Departmental Representative within the Node CECAM-IT-SAPIENZA<br>( <a href="http://www.cecarn.org/node_sapienza.html">http://www.cecarn.org/node_sapienza.html</a> ) |
| 2014-2017    | Management Committee Member for the Cluster funded by "Progetti Grandi Attrezzature 2013" from "Sapienza" Università di Roma.  |
| 2020-present | Responsible teacher of "Laboratorio di Calcolo" (Computing Lab)  |

Scientific Visits and Summer Schools	13 - 17 June 2011	Visit at the École Polytechnique Fédérale de Lausanne (EPFL) Lausanne, Switzerland Invited by Prof. Giuseppe Foffi
	7 - 12 June 2010	Visit at the École Polytechnique Fédérale de Lausanne (EPFL) Lausanne, Switzerland Invited by Prof. Giuseppe Foffi
	4 - 9 May 2009	Visit at the École Polytechnique Fédérale de Lausanne (EPFL) Lausanne, Switzerland Invited by Prof. Giuseppe Foffi
	2 - 7 September 2007	Visit at the École Polytechnique Fédérale de Lausanne (EPFL) Lausanne, Svizzera Invited by Prof. Giuseppe Foffi
	01/12/06- 31/01/07	Visit at the École Polytechnique Fédérale de Lausanne (EPFL) Lausanne, Svizzera Invited by Prof. Giuseppe Foffi
	8 - 11 August 2006	Visit at the École Polytechnique Fédérale de Lausanne (EPFL) Lausanne, Svizzera Invited by Prof. Giuseppe Foffi
	24 - 27 April 2006	Visit at the Department of Physics, University of Konstanz, Konstanz, Germany Invited by Prof. Matthias Fuchs
	26/02/06- 03/03/06	Visit at ESRF Grenoble Grenoble, France Invited by Prof. Stefano Mossa
	10 - 21 September 2001	Participation to Summer School: <i>10th Summer school of parallel computing</i> CINECA Bologna, Italy
	1-10 July 2001	Participation to Summer School: <i>"Methods in Molecular Simulations"</i> UMIST, Manchester, UK
Thesis Supervision	2024	Master in Physics - Tommaso Temperini ( <b>110/110</b> )
	2023	Bachelor in Physics - Theodore Manopulo
	2023	Master in Physics - Alessandro Forina ( <b>110/110 cum laude</b> )
	2022	Master in Physics - Giorgio Contestabile
	2022	Master in Physics - Mattia Trapella ( <b>110/110</b> )
	2021	Master in Physics - Simone Milano
	2021	Bachelor in Physics - Francesco Minati
	2020	Master in Physics - Carlo Andrea De Fiippo ( <b>110/110</b> )
	2018	Bachelor in Physics - Paolo Luigi Rinaldi ( <b>110/110 cum laude</b> ) Title: <i>"Uso delle reti neurali e del deep learning per la classificazione di strutture locali di particelle di forma sferica o anisotropa"</i>
	2017	Master in Physics - Alberto Giacomo Orellana ( <b>110/110 cum laude</b> ) Title: <i>"DNA-based liquid crystals: modeling and computer simulations"</i>
		Bachelor in Physics - Francesco De Cunzio Title: <i>"Integrazione Termodinamica Numerica"</i>
		Bachelor in Physics - Carlo Andrea De Filippo Title: <i>"Modellizzazione e simulazione di nanoparticelle di DNA"</i>
		Master in Physics - Emanuele Romani ( <b>110/110</b> ) Title: <i>"Proprietà elastiche di cristalli liquidi nematici ottenuti tramite autoaggregazione:"</i>

*simulazioni numeriche e teoria"*

- 2015 Bachelor in Physics - Valerio Di Giulio (**110/110 cum laude**)  
Title: "*Contributi elettrostatici alla teoria di Onsager nel caso di doppie eliche di DNA*"
- Bachelor in Physics - Giulio D'Acunto  
Title: "*Teoria di Parsons-Lee sulla transizione di fase isotropica-nematica*"
- 2014 Bachelor in Physics - Federico Stramaglia  
Title: "*Wertheim Theory for Sticky Hard Cylinders*"
- Bachelor in Physics - Massimiliano Proietti  
Title: "*Onsager Theory of Liquid Crystals*"
- 2013 Master in Physics - Daniele Ancora (**110/110**)  
Title: "*Aggregazione di Doppi Filamenti di DNA: Ruolo della Conformazione della Struttura a Doppia Elica*"

- Supervision of PhD Students
- 2011 - 2014 Khan Thuy Nguyen  
Project Title: "*Numerical Study of Short DNA Duplexes Self-Assembly*"
- 2021-2024 Carlo Andrea De Fiippo (co-supervised with Prof. B. Capone - UniRoma3)
- 2021-2024 Luca Bertini (co-supervised with A. Paciaroni of UniPg)
- 2023-present Mattia Trapella (co-supervised with Prof. A. Paciaroni UniPg)
- Supervision of Postdoc
- 2013 - 2014 Dott. Anna Battisti  
Project Title: "*Full-atom simulations of end-to-end aggregation of DNA and of Beta-lactoglobulin fibrils formation*".
- 2021 Benedetta Petra Rosi (co-supervised with Prof. A. Paciaroni e Dr. Lucia Comez)
- 2023 Deniz Mostarac
- 2023 Luca Bertini