

*Annual Report*  
*a.a. 2010-2011*

UNIVERSITÀ DELLA CALABRIA



Dipartimento di FISICA

ANNUAL REPORT 2011

*ACADEMIC YEAR 2010-2011*

*Scientific publications in 2011*

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## **DEPARTMENTAL ADMINISTRATION**

### **Head of Department:**

Pierluigi VELTRI

### **Executive Board:**

Riccardo BARBERI, Rosina BARTUCCI, Assunta BONANNO, Vincenzo FORMOSO, Alessandro PAPA , Nicola SCARAMUZZA, Giancarlo SUSINNO, Pierluigi VELTRI

### **Department Council:**

12 Full Professors

18 Associate Professors

23 Senior Researchers

9 Representatives of Post-Doctoral Research Fellows

13 Representatives of PhD students

5 Representatives of the Technical and Administrative Staff

### **Administrative Secretary:**

Gaspare PECORA

RESEARCH PERMANENT STAFF

**Full Professors**

1. Riccardo BARBERI *FIS/07*
2. Roberto BARTOLINO *FIS/07*
3. Vincenzo CARBONE *FIS/07*
4. Elio COLAVITA *FIS/07*
5. Giovanni FALCONE *FIS/01*
6. Roberto FIORE *FIS/02*
7. Ignazio GUERRA *GEO/10*
8. Antonino OLIVA *FIS/01*
9. Luigi SPORTELLI *FIS/07*
10. Giancarlo SUSINNO *FIS/01*
11. Cesare UMETON *FIS/01*
12. Pierluigi VELTRI *FIS/03*

**Associate Professors**

1. Raffaele AGOSTINO *FIS/01*
2. Rosina BARTUCCI *FIS/07*
3. Assunta BONANNO *FIS/01*
4. Lorenzo CAPUTI *FIS/01*
5. Enzo CAZZANELLI *FIS/03*
6. Gennaro CHIARELLO *FIS/07*
7. Gabriella CIPPARRONE *FIS/03*
8. Giovanni CROSETTI *FIS/01*
9. Laura LA ROTONDA *FIS/01*
10. Francesco MALARA *FIS/01*
11. Alessandro PAPA *FIS/02*
12. Francesco PIPERNO *FIS/03*
13. Nicola SCARAMUZZA *FIS/07*
14. Marco SCHIOPPA *FIS/01*
15. Enrico TASSI *FIS/01*
16. Carlo VERSACE *FIS/01*
17. Fang XU *FIS/01*
18. Gaetano ZIMBARDO *FIS/06*

**Senior Researchers**

1. Vincenzo BRUNO *FIS/07*
2. Michele CAMARCA *FIS/01*
3. Marcella CAPUA *FIS/01*
4. Roberto CAPUTO *FIS/03*
5. Tommaso CARUSO *FIS/07*
6. Anna CUPOLILLO *FIS/01*
7. Antonio DE LUCA *FIS/07*
8. Maria DE SANTO *FIS/07*
9. Vincenzo FORMOSO *FIS/01*
10. Domenico GIULIANO *FIS/02*
11. Antonella GRECO *FIS/07*
12. Rita GUZZI *FIS/07*
13. Fabio LEPRETI *FIS/03*
14. Anna MASTOBERARDINO *FIS/01*
15. Daniela PACILE' *FIS/01*
16. Pasquale PAGLIUSI *FIS/07*
17. Francesco PLASTINA *FIS/01*

18. Leonardo PRIMAVERA *FIS/05*
19. Pierfrancesco RICCARDI *FIS/01*
20. Marco ROSSI *FIS/02*
21. Antonello SINDONA *FIS/01*
22. Giuseppe STRANGI *FIS/07*
23. Francesco VALENTINI *FIS/03*

**Post-Doctoral Research Fellows**

1. Francesco CAPORALE
2. Enrico MACCALLINI
3. Giuseppina NIGRO
4. Marco ONOFRI
5. Barbara ORECCHIO
6. Valentino PINGITORE
7. Daniela SALVATORE
8. Sergio SERVIDIO
9. Tommaso VENTURELLI

**Phd School "Science, Communication and Technologies": Curriculum "Physics and Quantum Technology"**

1. Gennaro CORTESE (*XXIV Cycle*)
2. Silvio PIERRO (*XXIV Cycle*)
3. Giacinto CIAPPETTA (*XXV Cycle*)
4. Vincenzo LAVORINI (*XXV Cycle*)
5. Beatrice MURDACA (*XXV Cycle*)
6. Michele PISARRA (*XXV Cycle*)
7. Valentina CAPUTI (*XXVI Cycle*)
8. Angela MILAZZO (*XXVI Cycle*)
9. Amedeo PERRI (*XXVI Cycle*)
10. Diana RENZELLI (*XXVI Cycle*)
11. Valentina SANTOPAOLLO (*XXVI Cycle*)

**Phd School "Science and Technique": Curriculum "Physics of Complex Systems"**

1. Serena DALENA (*XXIV Cycle*)
2. Antonio Raimondo MARINO (*XXIV Cycle*)
3. Antoniou MYRSINI KYRIAKI (*XXIV Cycle*)
4. Giuseppe NISTICO' (*XXIV Cycle*)
5. Vincenzo CAPPARELLI (*XXV Cycle*)
6. Denise PERRONE (*XXV Cycle*)
7. Silvia SALSONE (*XXIV Cycle*)
8. Enrico Maria TROTTA (*XXV Cycle*)
9. Loris D'ALESSI (*XXVI Cycle*)
10. Gaetano DE VITA (*XXVI Cycle*)
11. Christian Natale GENCARELLI (*XXVI Cycle*)

**Phd School "Science and Technique": Curriculum "Science and Technologies of Mesophases and Molecular Materials"**

1. Fabio COSENZA (*XXIV Cycle*)
2. Giuseppe PUCCI (*XXIV Cycle*)
3. Silvia SALSONE (*XXIV Cycle*)
4. Angela FASANELLA (*XXV Cycle*)
5. Raul Josuè HERNANDEZ (*XXV Cycle*)
6. Manuela CATALANO (*XXVI Cycle*)
7. Ugo CATALDI (*XXVI Cycle*)
8. Eugenio LE PERA (*XXVI Cycle*)
9. Riccardo MASSARELLI (*XXVI Cycle*)
10. Alireza RASHIMI RASHED (*XXVI Cycle*)
11. Caterina TONE (*XXVI Cycle*)

## TECHNICAL AND ADMINISTRATIVE STAFF

### **Administration**

1. Gaspare PECORA (*Administrative Secretary*)
2. Lidia MAIDA
3. Anna Eduardina PASTORE

### **Secretary**

4. Luigina DE ROSE
5. Luigi PARISE
6. Francesco SCIOMMARELLA

### **Teaching Laboratories**

7. Mario LOMBARDI
8. Francesco PELLEGRINO

### **Computer Staff**

9. Nicola GUARRACINO (*Person in charge*)
10. Fedele STABILE

### **Research Laboratories**

*Ion-Matter Interaction and Surface Electronic Spectroscopy*

11. Vito FABIO

*Elementary Particles*

12. Paola TURCO

*Geophysics Laboratory*

13. Gerolamo LATORRE
14. Lorenzo FESTA

### **Mechanic's workshop**

15. Eugenio LI PRETI (*Person in charge*)
16. Vittorio ROMANO

The Physics Department hosts a INFN Section with the following staff:

Sonia VIVONA (*Administrative Official - INFN*)

Antonio BOZZARELLO (*Administrative Collaborator*)

**Department phonebook**  
(for calls from outside the Department, dial first (+39)-0984 -49)

INTERNET: @FIS.UNICAL.IT  
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AGOSTINO Raffaele	6162	PECORA Gaspare	6005
BARBERI Riccardo	6118-6150	PELLEGRINO Francesco	6102-6098
BARTOLINO Roberto	6122	PIPERNO Franco	6058
BARTUCCI Rosina	6074-6073	PLASTINA Francesco	6046
BONANNO Assunta	6170-6178	PRIMAVERA Leonardo	6138
BOZZARELLO Antonio	6008	RICCARDI Pierfrancesco	6171-6178
BRUNO Vincenzo	6043	SCARAMUZZA Nicola	6113-6151
CAMARCA Michele	6172-6178	ROMANO Vittorio	6106
CAPUA Marcella	6022	ROSSI Marco	6020
CAPUTI Lorenzo	6154-6173	SCHIOPPA Marco	6017-6104
CAPUTO Roberto	6124	SCIOMMARELLA Francesco	6011
CARBONE Vincenzo	6131-6033	SINDONA Antonello	6059
CARUSO Tommaso	6095	SPORTELLI Luigi	6076-6073
CAZZANELLI Enzo	6114-6142	STABILE Fedele	6027
CHIARELLO Gennaro	6157-6174	STRANGI Giuseppe	6120
CIPPARRONE Gabriella	6115-6148	SUSINNO Giancarlo	6016-6104
COLAVITA Elio	6156-6174	TASSI Enrico	6038
CROSETTI Giovanni	6021	TURCO Paola	6104
CUPOLILLO Anna	6160-6174	UMETON Cesare	6117-6152
DE LUCA Antonio	6124	VALENTINI Francesco	6129
DE ROSE Luigina	6001	VELTRI Pierluigi	6136-6033
DE SANTO Maria Penelope	6150	VERSACE Carlo	6116-6147
FORMOSO Vincenzo	6161	VIOLINI Galileo	6024
GIULIANO Domenico	6025	VIVONA Sonia	6007
GRECO Antonella	6132	XU Fang	6168-6178
GUARRACINO Nicola	6030	ZIMBARDO Gaetano	6134-6033
GUERRA Ignazio	3666		
GUZZI Rita	6077-6073		
LA ROTONDA Laura	6014-6102	<i>Network and Computer Service</i>	<i>6035</i>
LATORRE Gerolamo	3664	<i>Geophysics Laboratory</i>	<i>6068</i>
LE PRETI Fabio	6032	<i>Astrophysical Plasmas Computer Lab.</i>	<i>6033</i>
LI PRETI Eugenio	6179-6165	<i>Ion-Matter Interaction Lab.</i>	<i>6178</i>
LOMBARDI Mario	6083	<i>Electronic Spectroscopy Lab.</i>	<i>6174</i>
MAIDA Lidia	6006	<i>Biophysics Lab.</i>	<i>6073</i>
MALARA Francesco	6135-6033	<i>Molecular Physics Lab.</i>	<i>6151</i>
MASTROBERARDINO Anna	6031	<i>Particle Physics Lab.</i>	<i>6104</i>
OLIVA Antonino	6167-6178	<i>Mechanical Workshop</i>	<i>6106</i>
PACILE' Daniela	6164		
PAGLIUSI Pasquale	6148		
PAPA Alessandro	6015		
PARISE Luigi	6002		



## SEMINARS (2011)

*Feb 18, 2011*

Dr. Jyrki Piilo, University of Turku (Finland)  
*Markovianity and non-Markovianity in Quantum Mechanics*

*Feb 22, 2011*

Dr. Roberta Zambrini, Instituto de Fisica Interdisciplinar y Sistemas Complejos, Universitat Illes Balears  
*Quantum correlations in optical systems*

*Feb 18, 2011*

Dr. Jyrki Piilo, University of Turku (Finland)  
*Markovianity and non-Markovianity in Quantum Mechanics*

*Apr 18, 2011*

Dr. Kazumasa A. Takeuchi  
*Turbulent liquid crystals uncover universal behavior of macroscopic systems out of equilibrium*

*Jun 14, 2011*

Dr. Karen Volke Sepulveda  
*Micromanipulation of particles with periodic optical potentials*

*Jun 15, 2011*

Dr. Karen Volke Sepulveda  
*Angular momentum in rotating wavefield*

*Jun 30, 2011*

Dr. Dariia Lysenko - Institute of Physics, national Academy of Science of Ukraine  
*Strong Optical Nonlinearity of Gold nanoparticles Suspension in Nematic Liquid Crystal*

*Jul 6, 2011*

Dr. Gabriele Campagnano  
*Two-Particle interferometry with Anyons*

*Jul 20, 2011*

Dr. Barbara Kilosanidze  
*Integral Polarization–Holographic Element for Real-time Complete Analysis of the Polarization State of Light*

*Sep 28, 2011*

Prof. Derek Marsh  
*Fluid-fluid phase separation in cholesterol-containing membranes: rafts and non-rafts*

*Oct 6, 2011*

Prof. Vittorio de Giorgio, Facolta' di Ingegneria di Pavia - Prof. Mario Corti, facolta' di medicina di Milano  
*Aspetti di base della soft-matter, con risvolti nella biologia e medicina e nelle telecomunicazioni*

*Oct 27, 2011*

Prof. M. Paternostro, Queen's University, Belfast  
*Controllo quantistico di sistemi optomeccanici in cavita'*

*Nov 4, 2011*

Dr. Sergey Savin, Space Research Institute, Mosca  
*Super fast plasma streams as drivers of anomalous magnetopause transport and dynamics*

*Nov 11, 2011*

Dr. Luis Martin - Universidad de Buenos Aires (Argentina)  
*Impact of the Hall effect in a strong magnetic field*

Nov 28, 2011

Dott. Luis Martin - Universidad de Buenos Aires (Argentina)  
*Compressible and reduced Hall magnetohydrodynamics (Part I)*

Nov 29, 2011

Dott. Luis Martin - Universidad de Buenos Aires (Argentina)  
*Compressible and reduced Hall magnetohydrodynamics (Part II)*

Nov 15, 2011

Dr. Francesco Vissani  
*Osservazioni di neutrino, caratteristiche delle loro interazioni e masse*

Nov 16, 2011

Dr. Francesco Vissani  
*Fenomenologia delle oscillazioni di neutrino*

Nov 16, 2011

Dr. Francesco Vissani  
*Verifiche del numero leptonico totale*

Nov 17, 2011

Dr. Francesco Vissani  
*Neutrini in teorie di gauge*

Dec 1, 2011

Dr. Alexander Milovanov, ENEA - Centro Ricerche Frascati  
*The challenge of "complex" systems, with an implication of Fusion Advanced Studies Torus (FAST) project*

Dec 19, 2011

Prof. Michele Caselle, Università di Torino & INFN-Torino  
*Effective string models for confining gauge theories*

Dec 21, 2011

Dr. Pietro Giudice, Swansea University  
*Lattice Planar QED in external magnetic field as nonperturbative approach to the Quantum Hall Effect in Graphene*

Dec 20, 2011

Prof. G. Adesso (University of Nottingham)  
*Quantum correlations beyond entanglement: concept and measures*

Dec 21, 2011

Prof. G. Adesso (University of Nottingham)  
*Quantum correlations versus entanglement in composite systems*

Dec 22, 2011

Prof. G. Adesso (University of Nottingham)  
*Quantum correlations without entanglement: applications and perspectives*

Dec 22, 2011

Dr. N. Lo Gullo, University College Cork  
*Sensing quantumness with ultracold atoms*

## **LAUREA THESIS' in 2011**

### **1st LEVEL DEGREE THESIS' IN 2011**

#### **May 10**

Davide SCALISE

*Dinamica diffusiva dei bright point sulla fotosfera solare*

Relatore: Fabio LEPRETI

Rossella CIRILLO

*Produzione e caratterizzazione di carbonio attivato nanoporoso ad alta superficie specifica a partire da cellulosa microcristallina per applicazioni nello stoccaggio di metano*

Relatore: Raffaele Giuseppe AGOSTINO

Francesco GULLACE

*Verifica di alcune ipotesi per l'introduzione della fenomenologia dello TSUNAMI in un modello ad automi cellulari per frane sabaeree/subacquee*

Relatore: Salvatore DI GREGORIO

#### **July 26**

Tommaso ALBERTI

*L'influenza della radiazione solare sulla stabilità del clima terrestre*

Relatore: Vincenzo CARBONE

Oresta PEZZI

*Identificazione di vortici in turbolenze 3D*

Relatore: Vincenzo CARBONE, Sergio SERVIDIO

#### **July 27**

Angelo CURCIO

*Fantoccio per dosimetria EPR*

Relatore: Anna SANTANIELLO, Rita GUZZI, Roberto SICILIANO

Vincenzo CATANZARO

*Zincoporfirine in celle fotovoltaiche ibride*

Relatore: Raffaele AGOSTINO

#### **Sep 27**

Vera DI CIANNI

*Turbolenza nel vento solare*

Relatore: Vincenzo CARBONE

Tiziana RITACCO

*Proprietà collettiva della grafene su Pt (111)*

Relatore: Elio COLAVITA, Gennaro CHIARELLO

Gianluca FRANCIKA

*Decoerenza senza dissipazione in sistemi di Spin*

Relatore: Francesco PLASTINA

#### **Dec 13**

Francesca VITTORIOSO

*Effetti di TSUNAMI nel Mediterraneo*

Relatore: Vincenzo CARBONE

Paolo PUPO

*Risposta non lineare delle maree nei bacini chiusi: un modello di oscillazione di Helmholtz*

Relatore: Vincenzo CARBONE

Barbara FALBO

*Processi di rilassamento nell'atmosfera terrestre e struttura degli uragani*

Relatore: Vincenzo CARBONE

Claudia GIOIOSO

*Analisi e localizzazione di "Flux Ropes" nella turbolenza del vento solare*

Relatore: Vincenzo CARBONE

Marilisa ROMITO

*Realizzazione e caratterizzazione di strutture optofluidiche elettrocommutabili*

Relatore: Cesare UMETON

Serena PALAZZO

*Analisi dati raccolti con il calorimetro adronico dream*

Relatore: Laura LA ROTONDA

Valentina CARNEVALE

*Una derivazione lagrangiana per le equazioni di deriva cinetiche*

Relatore: Pierluigi VELTRI

Valentina, Maria Martina CAIRO

*Studi di calibrazione e data quality per lo spettrometro per muoni dell'esperimento ATLAS*

Relatore: Enrico TASSI

Flaviovincenzo QUARANTA

*Dosimetria EPR accidentale: il caso del saccarosio*

Relatore: Anna SANTANIELLO

Oreste DE LUCA

*Spettroscopia fotoelettronica a raggi X (XPS) su molecola di zinco-tetrafenilporfirine (ZNTPP) depositate su un substrato di ossido di titanio nanostrutturato*

Relatore: Agostino RAFFAELE

Emanuele MENDICELLI

*Periodicità classica e quantistica per la buca di potenziale infinita*

Relatore: Marco ROSSI

Mario LONGO

*Effetto Hall su grafene*

Relatore Alessandro PAPA

## **2st LEVEL DEGREE THESIS' IN 2011**

### **May 11**

Dario STELITANO

*Profer orthogonal decomposition di campi di radianze nell'infrarosso per l'interpretazione di immagini telerivelate*

Relatore: Vincenzo CARBONE

Francesca DI MARE

*Simulazioni numeriche per un modello di arco coronale con stratificazione di densità*

Relatore: Francesco MALARA

Luisa LIJOI

*Intermittenza nella turbolenza del vento solare: il modello di cascadeing*

Relatore: Luca SORRISO-VALVO

### **Jul 27**

Valerio SCARFONE

*Studio della produzione dei bosoni vettori W nella interazione protone-protone ad LHC*

Relatore: Enrico TASSI

Michele CARRIERO

*Hidrogen adsorption on novel 3D nanostructured carbon materials*

Relatore: Raffaele Giuseppe AGOSTINO

**Oct 4**

Antonia MORABITO

*La produzione del bosone Z nelle interazioni protone-protone ad LHC*

Relatore: Enrico TASSI

Antonio DE LIGUORO

*Fasi non convenzionali del modello di Hubbard su reticolo esagonale*

Relatore: Domenico GIULIANO

Claudia ROSSI

*Turbolenza nel vento solare a piccola scala*

Relatore: Vincenzo CARBONE

**Dec 14**

Stefania EVOLI

*Dinamica molecolare simulata in cupredoxine chimeriche*

Relatore: Rita GUZZI, Bruno RIZZUTO

Caterina TONE

*Studio di membrane di copolimeri a blocco con tecniche di microscopia a forza atomica*

Relatore: Maria Penelope DE SANTO

Ilaria BONETTI

*Preparazione e studio della risposta all'irraggiamento di materiali EPR sensibili drogati con atomi metallici per gli impieghi dosimetrici alle basse dosi*

Relatore: Anna SANTANIELLO, Rita GUZZI

Cristina LABATE

*Protein amyloid fibrillation studied by Atomic Force Microscopy*

Relatore: Maria Penelope DE SANTO, Bruno ZAPPONE

Marco CAPUTO

*Caratterizzazione spettroscopica e strutturale di Picene e Picene drogato con metallic alcalini*

Relatore: Gennaro CHIARELLO

Stefania STUCCI

*Realizzazione di un calorimetro a piccolo angolo per la misura della sezione d'urto  $e^+ e^- \rightarrow HYISR$  con l'esperimento BESIII all'acceleratore BEPCII*

Relatore: Marco SCHIOPPA

**PhD THESIS' in 2010**

(24° Cycle)

Serena D'ALENA

*Non-adiabatic particle transport in numerical models of turbulence*

Supervisore: Gaetano ZIMBARDO, Antonella GRECO, William H. MATTHAEUS

(24° Cycle)

Giuseppe NISTICO'

*Dynamics and evolution of solar corona: STEREO observations of jets, CMEs and numerical modeling*

Supervisore: Gaetano ZIMBARDO

(24° Cycle)

Antoniou MYRSINI KYRIAKI

*Methane Physisorption Processes on Porous Nanostructured Materials*

Supervisore: Raffaele Giuseppe AGOSTINO

(24° Cycle)

Antonio Raimondo MARINO  
*Electronic and Vibrational properties of ultrathin layers absorbed on metal surface*  
Supervisore: Gennaro CHIARELLO

(24° Cycle)  
Giuseppe PUCCI  
*Two phenomena of self-adaptation in out-of-equilibrium systems*  
Supervisore: Riccardo BARBERI, Yves COUDER

(24° Cycle)  
Salvatore LORENZO  
*Quantum State Transfer and Non-Markovian Dynamics*  
Supervisore: Francesco PLASTINA

(24° Cycle)  
Silvio PIERRO  
*Investigation of dimensionality effects on capacitorless memory and trench power MOSFET*  
Supervisore: Antonello SINDONA

(24° Cycle)  
Gennaro CORTESE  
*Critical properties of two-dimensional  $Z(N)$  vector models for  $N > 4$*   
Supervisore: Alessandro PAPA

## 1. ASTROPHYSICS

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Gaetano De Vita  
Luca Tiriolo

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## Introduction

The research in Astrophysics in the Physics Department of University of Calabria is mainly devoted to study plasma physics. Most of interplanetary matter and of the solar atmosphere is actually formed by plasma. For that reason, most of data obtained in space missions, or by solar observatories, can be interpreted within the framework of plasma physics. Such data have allowed for the construction of models describing astrophysical phenomena, and they have represented a powerful tool of investigation which has often given new perspectives for the comprehension of phenomena in fundamental physics. This has allowed to use the space as a huge laboratory where measurements not accessible in a terrestrial laboratory can be performed. On the other hand, using analogue techniques both on space and on laboratory measures allows for a comparison of the basic physical phenomena that take place on completely different scales, and for a comprehension of such phenomena which are relevant both in the domain of controlled thermonuclear fusion and in the perspective of industrial applications.

The group of Astrophysical Plasmas of Calabria University has been involved in such kind of problems, in collaboration with other groups of Italian universities (Pisa; Milano) and with Italian Institutions (IFSI - CNR of Frascati; Osservatorio Astrofisico di Arcetri; Consorzio RFX of Padova; INFN Milano) and foreign Institutions (Observatoire de Paris-Meudon, France; Université de Franche-Comte, Besancon, France; Goettingen University, Germany; Max-Planck-Institut für Sonnensystemforschung, Katlenburg-Lindau, Germany; International Space Science Institute, Bern, Switzerland; University of Innsbruck, Austria; Universitat Politècnica de Catalunya, Barcelona, Spain; University of Ioannina, Greece; Space Research Institute, Russia; Tbilisi University, Georgia; Bartol Research Institute, Newark, Delaware, USA; University of Delaware, Newark, USA; NASA Goddard Space Flight Center, Greenbelt, MD, USA; West Virginia University, USA; National Center for Atmospheric Research, Boulder, Colorado, USA; Dartmouth College, Hanover, New Hampshire, USA; Michigan State University, East Lansing, USA; Big Bear Solar Observatory, USA; Universidad de Buenos Aires, Argentina; University of Waikato, New Zealand).

The specific research themes under study during the year 2011 are described in the following.

### 1.1 MAGNETOHYDRODYNAMIC TURBULENCE AND KINETIC EFFECTS IN THE INTERPLANETARY SPACE

#### *Magnetic reconnection in turbulence*

Magnetic reconnection is a nonlinear process that occurs in many space, astrophysical, and laboratory systems. The underlying common feature for these systems is the presence of an inhomogeneous magnetic field that changes rapidly across a very narrow region. Generally, a strong peak in the electric current density is present. Reconnection implies the presence of a magnetic X-type neutral point in two-dimensions (2D), and more generally a change in magnetic topology resulting in the conversion of magnetic into kinetic energy. Since it might occur in any region separating topologically distinct magnetic flux structures, reconnection might be expected to be of importance in more general circumstances, including magnetohydrodynamic (MHD) turbulence. Very high resolution numerical simulations of 2D MHD turbulence reveal the presence of a large number of X-type neutral points where magnetic reconnection occurs. In this scenario, reconnection is spontaneous, but locally driven by the fields and boundary conditions provided by turbulence itself. Because of the complex magnetic topology, turbulence leads to different kinds of reconnecting patches. In contrast with laminar reconnection models that provide a single predicted reconnection rate for the system, turbulent resistive MHD gives rise to a broad range of reconnection rates that depend on local turbulence parameters.



Many potential reconnection sites are present, but only a few are selected by the turbulence, at a given time, to display robust reconnection electric fields. In this way, the present problem differs greatly from studies of reconnection that assume that it occurs in isolation. In turbulence the associated reconnection rates are distributed over a wide range of values and scales with the geometry of the diffusion region. Locally, these events can be described through a variant of the Sweet-Parker model, in which the parameters are externally controlled by turbulence. This new perspective on reconnection is relevant in space and astrophysical contexts, where plasma is generally in a fully turbulent regime.

#### ***Local processes in MHD turbulence and non-Gaussian statistics***

Two central features of magnetohydrodynamic (MHD) turbulence are generally studied independently: the production of intermittency and the appearance of distinctive states associated with turbulent relaxation. It is, for example, well known that the random phase approximation fails as a turbulence description in that it cannot produce non-Gaussian statistics, such as high kurtosis of vorticity and current, multifractal scaling of moments, and other signatures of intermittency. On the other hand, MHD relaxation theory has led to notable successes associated with Taylor relaxation, selective decay, global dynamic alignment, and helical dynamo action.

Direct numerical simulations show that undriven MHD turbulence spontaneously generates coherent spatial correlations of several types, associated with local Beltrami fields, directional alignment of velocity and magnetic fields, and anti-alignment of magnetic and fluid acceleration components. These correlations suppress nonlinearity to levels lower than what is obtained from Gaussian fields, and occur in spatial patches. We suggest that this rapid relaxation leads to non-Gaussian statistics and spatial intermittency. To further confirm this scenario, we have performed spectral method simulations of ideal MHD, investigating the production of coherent small scale structures. The near-identical growth (in the initial stage) of non-Gaussianity in ideal and non-ideal cases suggests that generation of coherent structures and breaking of self-similarity are essentially ideal processes. This has important implications for understanding the origin of intermittency in turbulence.

#### ***Local relaxation and maximum entropy in two-dimensional turbulence***

The phenomenon of vortex merging in two-dimensional hydrodynamics has been investigated through direct numerical simulations. The fast and local processes that occur during the turbulent relaxation of a randomly initialized system in periodic geometry have been examined. The analysis reveals that many of the coherent structures can be described by a local principle of maximization of entropy. The validity of this entropy principle has been further confirmed by time-dependent statistics using a contour-tracking technique. Implications for the description of persistent coherent vortices commonly observed in nature are suggested, including growing evidence for the wide applicability of maximum entropy-based relaxation principles.

#### ***Kinetic processes in Vlasov Turbulence***

Strong turbulence, a difficult problem in fluid regimes, is an even more challenging subject in a kinetic, low collisionality, plasma. Plasma turbulence additionally involves wave-particle interactions that are responsible for crucial effects such as plasma dissipation, acceleration mechanisms, heating, temperature anisotropy and so on. We study these local kinetic processes using a hybrid-Vlasov numerical code, in a fully turbulent regime. Nearby regions of strong magnetic activity, evident kinetic effects manifest through a deformation of the distribution function. These departures from a equilibrium Maxwellian configuration may be responsible for the production of heating and anisotropy, commonly observed in many astrophysical turbulent systems.

#### ***Local anisotropy, "higher order" statistics and spectra in turbulence***

Correlation and spectral anisotropy play important roles in solar wind and astrophysical plasmas, having significant impact on descriptions of the turbulence cascade, particle scattering, the nature of kinetic dissipation, and the transport of turbulence. Anisotropy emerges dynamically in MHD, producing stronger gradients across the large-scale mean magnetic field than along it, and occurring both globally and locally. Recently, properties of correlation anisotropy have been investigated through numerical simulations, showing the effect is intensified for more localized estimates of the mean magnetic field. The mathematical formulation of this property shows that local anisotropy mixes second-order with higher order correlations. Sensitivity of local statistical estimates to higher order correlations can be understood in connection with the stochastic coordinate system inherent in such formulations. We demonstrate this in specific cases, and illustrate the connection to higher order statistics by showing the sensitivity of local anisotropy to phase randomization, after which the global measure of anisotropy is recovered at all scales of averaging. This study establishes that anisotropy of the local structure function is not a measure of anisotropy of the energy spectrum, but is rather related to higher order statistics.

#### ***Intermittent structures and magnetic discontinuities in MHD turbulence and solar wind***

We re-examine the statistics of rapid spatial variations of the magnetic field in simulations of Hall magnetohydrodynamic (HMHD) turbulence, using analysis of intermittency properties of the turbulence, and also using methods often employed to identify discontinuities in the solar wind (as in the earlier work of Tsurutani & Smith 1979). The hypothesis is that the statistics of intermittent events might be related to the statistics of classical MHD

discontinuities. Indeed, those methods give similar distributions of events, often identifying the same structures. This suggests that observed discontinuities might not be static solutions to the MHD equations, but instead may be related to the intermittent structures that appear spontaneously in MHD turbulence. Then, we further examine the link between intermittency and MHD discontinuities, directly comparing statistical analysis from solar wind data and 3D and 2D simulations of MHD turbulence. The comparison between ACE solar wind data and simulations of magnetohydrodynamic turbulence shows a good agreement in the Waiting-Time analysis of magnetic field discontinuities. This result adds to evidence that solar wind magnetic structures may emerge fast and locally from nonlinear dynamics that can be properly described in the framework of MHD theory.

Using high Reynolds number simulations of two-dimensional magnetohydrodynamic (2D MHD) turbulence as a test case, a statistical association between tangential discontinuities and magnetic reconnection is demonstrated. Methods employed in previous studies on discontinuities and reconnection in turbulence are used to identify sets of possible reconnection events along a one-dimensional path through the turbulent field, emulating experimental sampling by single detector in a high speed flow. The goal is to develop numerical algorithms for identifying candidate reconnection events in space physics applications. We find that sets of strong discontinuities, identified using the normalized partial variance of vector increments (PVI), include an increasing fraction of reconnection events as the threshold for identification grows. Magnetic discontinuities become almost purely reconnection events for high thresholds, with values generally higher than six standard deviations.

The formation of these coherent structures in turbulence is a signature of a developing cascade and therefore might be observable by analysis of inner heliospheric solar wind turbulence. To test this idea, data from the Helios 2 mission, for six streams of solar wind at different heliocentric distances and of different velocities, are subject to statistical analysis using the partial variance of increments (PVI) approach. We see a clear increase of the PVI distribution function versus solar wind age for higher PVI cutoff, indicating development of non-Gaussian coherent structures. The plausibility of this interpretation is confirmed by a similar behavior observed in two-dimensional magnetohydrodynamics simulation data at corresponding dimensionless nonlinear times.

#### ***Study on the Turbulent Magnetic Dynamo: A Self-consistent Nonlinear Model***

Magnetic fields are ubiquitous in our Universe: planets, stars, entire galaxies, black holes etc. all having associated magnetic fields. The most accredited mechanism which explains the generation and self-sustaining of a magnetic field is the so-called dynamo effect, i.e. the maintaining of a magnetic field against diffusive effects by the motion of electrically conducting fluids. One of the examples of dynamo effect closest of our experience is the presence of the Earth's magnetic field. Paleomagnetic measurements showed that the Earth's magnetic dipole reverses stochastically in time, with intervals ranging from  $10^4$  to  $10^7$  years. Many researchers have dealt with this problem using direct numerical simulations (DNS), even if realistic parameter regimes are beyond the power of actual supercomputers. Difficulties arise from the realistic description of both large-scales and small-scale (high Reynolds numbers) turbulence, which is responsible of dynamo effect. Actual DNS are able to simulate only some few polarity reversals of the magnetic field. To overcome these difficulties we have built a self-consistent nonlinear dynamo model, which can describe turbulent fluctuations at very large Reynolds numbers. In particular, our model couples the evolution of the large-scale magnetic field with turbulent dynamics of the plasma at small scales by electromotive force. We solve the induction equation, describing the time evolution of the large-scale magnetic field, in local approximation; while the turbulent dynamics at small scales is described by using a low-dimensional model (shell model). Turbulent fluctuations at small scales generate a dynamical situation in which the large-scale magnetic field randomly jumps between two states which represent the opposite polarity of the magnetic field. An important result of this research is related to the critical role that the turbulence plays in the dynamo effect. The model allows us to reproduce very long time series of reversals. The statistical study of these polarity reversals reveals, together with paleomagnetic data, the presence of long-time hidden correlations in the chaotic dynamo process, bringing to light some degree of memory in the history of the Earth's magnetic field.

#### ***The evolution of the solar wind turbulence at typical kinetic scales***

The interplanetary medium, the bubble of plasma that is generated by the Sun and that fills the Heliosphere, is known to be hotter than expected for an expanding, almost collisionless plasma. Understanding how energy from the Sun can be dissipated into heat in such a collision-free system represents a top priority in space physics. The Sun injects energy into the Heliosphere through large wavelength fluctuations, mainly in the form of Alfvén waves. This energy is then channeled towards short scales through a turbulent cascade until it can be transferred to the plasma particles in the form of heat. Turbulence is therefore thought to be responsible for the local heating of the solar wind and kinetic effects at short wavelengths are considered to be the best candidate in replacing collisional processes and in "dissipating" the energy coming from the large scales.

Nowadays, due to the impressive growth in computational resources, it is possible to investigate numerically the role of kinetic effects in the evolution of turbulence as well as in other basic processes, e.g. magnetic reconnection. In 2007 we introduced a new Eulerian hybrid-Vlasov model to analyze numerically the ion kinetic dynamics of a collisionless magnetized plasma. This numerical code integrates numerically the Vlasov equation for the proton

distribution function coupled to the Maxwell equations for the electromagnetic fields. Within this hybrid model, the electrons are considered as a fluid. Through this algorithm we succeeded in describing the evolution of the turbulent cascade in the solar wind going from large scales (somewhat larger than the ion skin depth) towards short wavelengths, in a phase space of reduced dimensionality (1D-3V, i. e. one dimension in physical space and three dimensions in velocity space). Moreover, recent simulations in a 2D-3V phase space configuration gave us important insights into the nature of the local and fast reconnection events occurring as the results of the turbulent cascade.

The results of these kinetic simulations lead to the identification of a new electrostatic wave channel (the so-called ion-bulk waves) available for the energy cascade to develop towards short wavelengths in the direction longitudinal to the background magnetic field. These waves have acoustic type dispersion, phase speed comparable to the proton thermal speed and can survive against Landau damping thanks to the presence of plateaus in the longitudinal particle velocity distribution. Due to the effect of this plateau, the ion-bulk waves, at variance with the well-known ion-acoustic waves, can survive against damping even for low values of the electron to proton temperature ratio, thus being robust even in typical conditions of the interplanetary medium.

The propagation of these fluctuations has been investigated in detail by making use of two different Vlasov codes. The first is an electrostatic Vlasov code, that allowed us to describe the plasma dynamics up to wavelengths of the order of the Debye length. The second is the hybrid Vlasov-Maxwell code mentioned above, which is limited by the quasi-neutrality assumption that rules out charge separation effects, but allowed us to analyze the link between large MagnetoHydrodynamics scales and kinetic scales. Moreover a new version of the hybrid Vlasov-Maxwell code has been realized to include the numerical integration of the Vlasov equation for alpha particles, a significant component of the solar wind plasma. Through this new version of the hybrid algorithm we were able to analyze the effect of heavy ions on the development of the solar wind cascade and to point out important effects such as the generation of temperature anisotropy both in the proton and in the alpha species, this begin a common feature frequently observed in "in situ" measurements from spacecraft.

## 1.2 OBSERVATIONS AND TURBULENCE MODELS IN THE SOLAR ATMOSPHERE

### *Propagation of gravity waves in the Sun*

The interior of the Sun behaves like a resonant cavity, supporting the excitation of global oscillations at discrete frequencies. In the presence of a gravitational field and density stratification, two kinds of oscillations can be excited, namely acoustic  $p$ -modes and gravitational  $g$ -modes. Since gravity modes are concentrated near the center of the Sun, they would be excellent probes to access the physics of the deep interior and their observation would represent a fundamental improvement for helioseismology. The possibility of detecting  $g$ -modes on the solar surface depends on their surface amplitudes, which are dependent on the energy of the modes generated in the solar interior and on their ability to cross the convection zone of the Sun. The difficulty of observing  $g$ -modes has usually been attributed to their difficulty in penetrating the convection zone. In fact, the linear theory predicts that  $g$ -modes become evanescent waves in a convectively unstable layer, so that their amplitudes should decrease exponentially through the convection zone. We performed numerical simulations of gravity mode propagation in a convective layer to investigate the observed association between small spatial scales and low frequencies in the photospheric velocity fields. According to the linear theory, when the fluid layer is convectively unstable, gravity modes are evanescent waves. However, in simple two-dimensional numerical settings, we find that when the equilibrium structure is modified by coherent large-scale convective motions, the waves injected at the bottom of the layer are no longer evanescent. In this situation, gravity waves can be detected at the surface of the layer. In our simplified model the injected wave's frequency remains unchanged, but its amplitude has a spatial modulation determined by the convective structure. This result may explain some analyses done with the proper orthogonal decomposition method of the solar surface velocity field.

### *Solar activity cycle*

The investigation of the main features of the solar cycle are essential in order to set parameters for theoretical dynamo models. The magnetic solar cycle consists of two components: the well-known main cycle with period around 22 yr, and a high-frequency component with period close to 2 yr, known as Quasi Biennial Oscillations (QBO). The spatio-temporal dynamics of the solar magnetic field has been investigated by using NSO/Kitt Peak synoptic magnetic maps covering the period August 1976-September 2003. Results obtained for the 22 yr cycle, mainly related to the polarity inversions of the large-scale dipolar field, show an antisymmetric behavior with respect to the equator and a marked poleward flux migration in the radial and meridional components. Our findings suggest a deep seated alpha effect and support alpha-omega dynamo models which also include meridional circulation. The quasi biennial oscillations are also identified as a fundamental periodicity of the magnetic field and linked to a dynamo action which possibly causes magnetic flux migration at  $\sim 2$  yr rate both polewards and equatorwards from low latitudes ( $-25^\circ$  and  $+25^\circ$  in the Southern and Northern hemisphere, respectively). In particular, the equatorwards drift is clearly found in the toroidal component and shows antisimmetry with respect to the equator. The reproducibility of these features represents a validation test of the theoretical dynamo models, developed to understand the spatio-temporal evolution of the solar magnetic field. The QBOs have been detected as a prominent scale of variability in CR data. The superposition of the 11

yr and QBO contributions reproduces the general features of the CR modulation, such as most of the step-like decreases and the Gnevyshev Gap phenomenon. A significant correlation has also been found between QBOs of the heliospheric magnetic field and the CR intensity during even solar activity cycles, suggesting that the former are responsible for step-like decreases in CR modulation, probably dominated by the particle diffusion/convection in such periods. In contrast, during odd-numbered cycles, no significant correlation is found. This could be explained with an enhanced drift effect also during the solar maximum or a greater influence of merged interaction regions at great heliocentric distances during odd cycles. Moreover, the QBOs of CR data are delayed with respect to sunspot activity, the lag being shorter for  $A > 0$  periods of even cycles (1–4 months) than for  $A < 0$  periods of odd cycles (7–9 months); we suggest that solar QBOs also affect the recovery of the CR intensity after the solar activity maximum.

#### ***Nonlinear development of current sheet instability for a solar coronal loop***

We investigated the dynamics of the coronal plasma in order to understand the physical mechanism responsible for nano-flares. Studying the dynamical behaviour of a current sheet in a plasma system with line-tied boundary conditions, we can relate the explosive plasma instability, which takes place in this framework, to the impulsive energy release thought to take place in a solar coronal loop. Within this interpretation, we want to investigate a basic situation in which the instability develops in a specific magnetic topology driven by a shearing velocity at the boundaries of the simulation box (top and bottom). Imposing a velocity shear at boundary, we expect the formation of current sheets which undergo a fragmentation after the saturation of the tearing modes and the secondary instability. In this case we expect also the formation of energy spectra (kinetic and magnetic energy spectra) with a power-law range with slope around two. The line-tied boundary condition however strongly restricts the plasma dynamics. We want to study closely this situation in order to understand how the energy which heats the corona is derived from stresses that have built up in the magnetic field. We solve the cold plasma MHD equations with a background homogeneous magnetic field neglecting loop curvature by using a new parallelized viscoresistive three-dimensional code. The code employs a Fourier collocation-finite difference spatial discretization, and uses a third-order Runge-Kutta temporal discretization.

#### ***Non diffusive propagation of solar energetic particles.***

The propagation of solar energetic particles encompasses a number of transport regimes, which goes from diffusive transport to scatter-free propagation. On the other hand, numerical simulations in the presence of magnetic turbulence, as well as the analysis of propagating particles accelerated at interplanetary shocks, show that superdiffusive regimes, which are intermediate between scatter free and diffusive propagation, can be found. In this work we study both proton and electron transport in order to understand whether both superdiffusive and ballistic propagation are indeed possible, at variance with the standard paradigm. We carry out an analysis of impulsive solar energetic particles (SEPs) events, for which the observed time profile of energetic particle fluxes represents the propagator of the corresponding transport equation. Time profiles are fitted by power laws. Assuming well-known forms of the particle propagator, with power-law asymptotic behaviour, we determine the transport regime of particle propagation from the time profiles. Using data obtained from ACE and SoHO spacecraft, several proton and electron events that exhibit both superdiffusive and ballistic transport have been found. When this is the case, no finite mean free path can be defined.

#### ***Coronal heavy ion reflection and heating by quasi-perpendicular collisionless shocks.***

We propose a new model for explaining the observations of preferential heating of heavy ions in the polar solar corona. We consider that a large number of small scale shock waves can be present in the solar corona, as suggested by recent observations of polar coronal jets by the Hinode and STEREO spacecraft. The heavy ion energization mechanism is, essentially, the ion reflection off supercritical quasi-perpendicular collisionless shocks in the corona and the subsequent acceleration by the motional electric field  $E = -V \times B$ . The acceleration due to the electric field is perpendicular to the magnetic field, giving rise to large temperature anisotropy with perpendicular temperature much larger than the parallel one, which can excite ion cyclotron waves. Also, heating is more than mass proportional with respect to protons, because the heavy ion orbit is mostly upstream of the quasi-perpendicular shock foot. The observed temperature ratios between  $O(5+)$  ions and protons in the polar corona, and between alpha particles and protons in the solar wind are easily recovered. We also identify the mechanism of heavy ion reflection, which is based on ion gyration in the magnetic overshoot of the shock. A test particle numerical simulation has been developed which allows to study the process of heavy ion reflection, showing that under typical conditions the rate of reflection of heavy ions is comparable to that of protons.

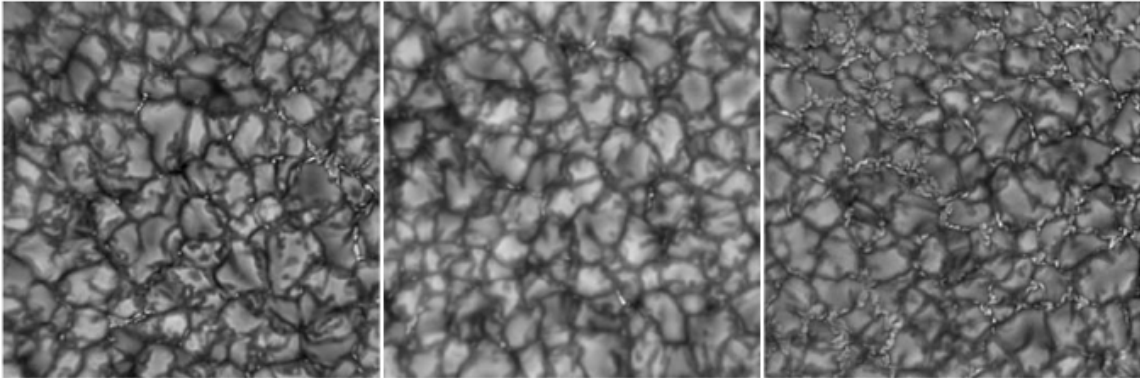
#### ***Plasma jets in the solar corona.***

Coronal hole jets are fast ejections of plasma occurring within coronal holes, observed at Extreme-UltraViolet (EUV) and X-ray wavelengths. Recent observations of jets by the STEREO and Hinode missions show that they are transient phenomena which occur at much higher rates than large-scale impulsive phenomena like flares and Coronal Mass Ejections (CMEs). In this research we describe some typical characteristics of coronal jets observed by the SECCHI instruments of STEREO spacecraft. We show an example of 3D reconstruction of the helical structure for a south pole jet. Then we discuss a temperature determination for the jet plasma by using the filter ratio method at 171

and 195 and applying a technique for subtracting the EUV background radiation. The results show that jets are characterized by electron temperatures ranging between 0.8 and 1.3 MK. We present the thermal structure of the jet as temperature maps and we describe its thermal evolution, which shows that the jets, and the associated magnetic reconnection, exist well before the main ejection phase. This work has given rise to a paper published on *Advances in Space Research* which has been awarded from COSPAR a prize for the best student paper.

### **Turbulent diffusion of photospheric bright points**

Understanding diffusion and transport of magnetic fields within the turbulent motions in the solar convection zone and atmosphere is of fundamental importance for several solar physics problems, such as dynamo, magnetoconvection, and energy release processes in the atmosphere. In this context, the motions of local magnetic flux concentrations and magnetic bright points (BPs) represent one of the main sources of information. On the basis of observations of solar granulation (Figure 1) obtained with the New Solar Telescope of Big Bear Solar Observatory, we explored the motions of BPs in a quiet-sun area, a coronal hole, and an active region plage.



*Figure 1. Photospheric granulation and magnetic bright points observed with the Big Bear Solar Observatory New Solar Telescope (BBSO/NST).*

We automatically detected and traced BPs and derived their mean-squared displacements as a function of time (starting from the appearance of each BPs for all available time intervals). In all three magnetic environments, we found the presence of a super-diffusion regime, which is the most pronounced inside the time interval of 10–300 s. Super-diffusion, measured via the diffusion exponent,  $\gamma$ , which is the slope of the mean-squared displacement spectrum, increases from the plage area ( $\gamma = 1.48$ ) to the quiet-sun area ( $\gamma = 1.53$ ) to the coronal hole ( $\gamma = 1.67$ ). We also found that the coefficient of turbulent diffusion changes in direct proportion to both temporal and spatial scales. For the minimum spatial scale (22 km) and minimum time scale (10 s), it is 22 and 19  $\text{km}^2 \text{s}^{-1}$  for the coronal hole and the quiet-sun area, respectively, whereas for the plage area it is about 12  $\text{km}^2 \text{s}^{-1}$  for the minimum time scale of 15 s. We applied our BP tracking code to three-dimensional MHD model data of solar convection and found the super-diffusion with  $\gamma = 1.45$ .

## **1.3 MAGNETOSPHERIC PHENOMENA AND GEOPHYSICS**

### ***Proton acceleration in the Earth's magnetotail***

Ion beams with energies of the order of several tens of keV are frequently observed in the Earth's magnetotail. In previous years we have developed a 2D test particle simulation where ions are accelerated by the interaction with moving clouds. In order to have a more realistic description of ion acceleration, a three-dimensional (3D) model which takes into account the magnetic structure of the current sheet has to be developed. In such a case the magnetic perturbations correspond well to the magnetic islands which are observed in the Earth's magnetotail. The main findings are: (a) the presence of a large scale magnetic field tends to decrease the efficiency of the Fermi-like interaction between test particles and moving clouds. (b) The ion energization grows with the (x, y) size of the magnetic clouds, while it is slightly influenced by the thickness of the clouds along z, implying that the majority of the interaction takes place in the (x, y) plane. (c) Assuming parameters of the model corresponding to those of the Earth's magnetotail, protons are accelerated to energies comparable to those observed in the plasma sheet boundary layer, and it is found that many features, like the formation of a beam in velocity space, can be reproduced.

In another study, we studied the role of intermittency in the process of acceleration and transport of charged particles by electromagnetic turbulence. We propose a simple model of electromagnetic turbulence with a variable level of intermittency. The magnetic field is described as a superposition of an ensemble of magnetostatic plane waves and of spatially localized dynamic magnetic clouds. The amplitudes of magnetic clouds are distributed according to an intermittent map. The model approximates essential properties of turbulence observed in situ in the neutral plane of the Earth's magnetotail. Numerical integration of charged particle trajectories in such a dynamic electromagnetic environment shows that, for the fixed time interval, the higher the level of intermittency, the higher the energy gain.

Moreover, in a sufficiently intermittent turbulence, particle acceleration occurs without significant intensification of the spatial transport.

### *Sun-Earth interactions*

The presence of long-term persistence in climate system is already debated. It is commonly investigated through the estimate of the detrended fluctuation analysis (DFA) scaling exponent  $\delta$ , representing a statistical index related to the dynamics of fluctuations of a stochastic process. Some Earth's temperature data sets showed the same degree of persistence with an exponent  $\alpha = 0.65$  in the range of time scales from 2 to 15 yr. More recently this sort of universality has been questioned since a value  $\alpha = 0.5$  seems to be present over continental lands while higher values  $\alpha = 0.65$  have been found over the coastline. In order to calculate the degree of persistence, we need to distinguish between trends and correlations. Usually, to eliminate trends in the temperature data sets, the temperature anomalies are calculated. In climate studies, these are defined as the difference between the temperature measured at a given day and the temperature mean value for the same calendar day over many years of data. In such a definition of anomaly, there is the implicit assumption that the seasonal annual cycle is constant, and it is generated by a set of stationary processes. Clearly, since the response of the climate system to external forcing, such as the solar one, is nonlinear, the validity of the previous assumption is often questionable. Hence, the classical definition of anomaly could not be adequate to the complex physics of the system; and, consequently, the persistence estimation. Because of the nonlinear and nonstationary character of temperature time series the seasonal contribution has been identified through a novel technique, the Empirical Mode Decomposition. This tool recovers a set of orthogonal empirical modes called IMFs. The anomalies have been thus obtained through partial reconstructions by excluding IMFs associated to obvious persistence effects such as the urban warming and the seasonal cycle. Results from monthly historical temperature records measured for about 250 yr in Prague and Milan indicate persistence on scales from 3 to 10 yr with similar values for the detrended fluctuation analysis indices thus indicating that a suitable definition of anomalies is fundamental when persistence effect in climate is investigated. The dynamics of the climate system has been investigated, through the EMD, by analyzing the seasonal oscillation of monthly averaged temperatures recorded at 1167 stations covering the whole USA. We found the presence of an orbit-climate relationship on time scales of about 20 yr related to the nutational forcing. The relationship manifests itself through occasional destabilization of the phase of the seasonal component due to the local changing of balance between direct insolation and the net energy received by the Earth. The local intermittent dynamics is modulated by a periodic component of 18.6 yr due to the nutation of the Earth, which represents the main modulation of the Earth's precession. The global effect in the last century results in a cumulative phase-shift of about 1.74 days towards earlier seasons, in agreement with the phase shift expected from the Earth's precession. The climate dynamics of the seasonal cycle has been described through a nonlinear circle-map, indicating that the destabilization process can be associated to intermittent transitions from quasi-periodicity to chaos.

### *Effects of far-generated tsunami in tidal spectra*

We investigated the possibility that the tsunami, generated as a consequence of the large Mw 9.0 Tohoku-Oki earthquake of March 11<sup>th</sup> 2011, could be recorded by the tide gauge stations located in the Mediterranean Sea. We find two kinds of transient signatures which should be attributed to the far-field destabilizing effect of the tsunami on the usual tidal components: 1) the excitation of a broad spectrum of frequency fluctuations, superimposed to the diurnal and semidiurnal tidal components, 2) the change of amplitude of the low-frequency tidal components in the Mediterranean, related to the sea surface fluctuation perhaps caused by the direct transmission of the tsunami across Gibraltar.

## **1.4 LABORATORY PLASMAS**

### *Compressible magnetohydrodynamic simulations of the Reversed Field Pinch*

A reversed field pinch is a toroidal configuration used to confine plasmas in fusion machines. The poloidal and toroidal components of the magnetic field in an RFP are mostly generated by electric currents flowing in the plasma and they are of the same order of magnitude. The configuration is characterized by a reversal of the toroidal magnetic field close to the wall. Besides the interest of this kind of machines as potential fusion reactors, they are also useful for the study of fundamental issues like plasma relaxation, plasma turbulence and its effects on plasma confinement. We studied the reversed field pinch through the numerical solution of the compressible magnetohydrodynamic equations.

Two kinds of compressible magnetohydrodynamics simulations of the reversed-field pinch have been performed, with isotropic and anisotropic thermal conductivity. We developed a numerical method to reproduce the effect of a large parallel thermal conductivity using a multiple-time analysis, which makes magnetic field lines almost isothermal. We showed that the anisotropic thermal conductivity causes the formation of a hot island when closed magnetic surfaces exist, while temperature becomes almost uniform when the magnetic field is chaotic. The simulations show the effects of the anisotropic thermal conductivity on the system evolution. Including the anisotropy in the thermal conductivity is necessary to obtain more reliable numerical results. The simulations show that single-helicity states in the reversed-field pinch are obtained when the resistivity has a radial profile sharply increasing close to the wall. In contrast, a uniform resistivity produces multiple-helicity states. A radially increasing resistivity profile is

determined in RFP experiments by the temperature difference between the plasma core and the wall. The results of the simulations presented are an indication that quasi-single-helicity states observed in experiments with high toroidal currents may be a consequence of the resistivity profile determined by the high temperatures reached in the plasma core in high-current discharges.

### **Turbulence in pure electron plasmas**

Electron plasmas confined in Penning-Malmberg traps evolve, in a wide range of operational parameters, as near-ideal 2D fluids with a single sign of vorticity. This provides the opportunity to perform experimental studies of 2D fluid dynamical processes such as shear flow instabilities, self-organization, vortex formation, and turbulence. We have studied dynamical and statistical properties of freely decaying 2D turbulence in pure electron plasmas by analyzing the results of experiments performed in the Penning-Malmberg trap ELTRAP. Different types of initial conditions, namely annular vorticity and spiral vorticity distributions, have been investigated. The role and evolution of coherent structures have been analyzed through the Proper Orthogonal Decomposition (POD) technique. A major concentration of the enstrophy in the first POD modes is found in the case of annular initial conditions. The empirical eigenfunctions (Figure 2) show coherent structures with a size of the order of 5–6 mm, which give a dominant contribution to the POD modes with the major enstrophy content.

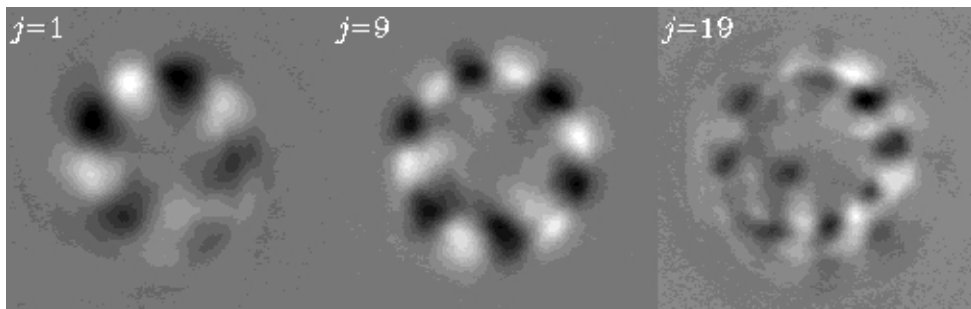


Figure 2. Empirical eigenfunctions of some of the dominant POD modes obtained from experiments of 2D turbulence of an electron plasma.

The time evolutions of the modal coefficients for these modes is characterized by regular oscillations. This behavior can be attributed to the emergence of the fastest growing diocotron modes originating from the initial annulus of vorticity. In the case of spiral initial conditions, the enstrophy is more equally distributed among the POD modes. The POD eigenfunctions show structures in a broader range of spatial scales, and more precisely the coexistence of large-scale, coherent vortices and a background of smaller-scale vorticity structures. The time evolution of the modal coefficients is dominated by stochastic fluctuations. These results indicate that spiral vorticity initial conditions give rise to a fairly developed turbulent cascade process. The intermittency properties of this turbulence have been studied by analyzing the scaling properties of vorticity increments. It has been shown that intermittency increases as turbulence develops, due to the formation of strong vorticity fluctuations which give rise to non-Gaussian tails in the PDFs of vorticity increments.

## **1.5 COMPLEX SYSTEMS**

### ***Instabilities and structuring effects in liquid crystals***

We studied the complex spatio-temporal dynamics generated by electrohydrodynamics instabilities in a nematic liquid crystal under the action of a driving oscillating electric field. Quasi-stationary convective structures at large scales are formerly created and, when the voltage is increased, are broken into chaotic patterns, thus generating small-scale structures. Scaling analysis reveals that these small-scale structures self-organize in a network of subleading structures which are reminiscent of convective rolls. This network persists well inside the chaotic regimes, disappearing only at very high voltages, where stochastic dynamical scattering mode takes place.

## A PUBLICATIONS ON SCIENTIFIC JOURNALS

### A.1 Publications on international journals

#### A.1.1 Publications on international journals printed in 2011

1. Valentini F., Califano F., Veltri P.,  
*The kinetic nature of turbulence at short scales in the solar wind*  
Journal of Geophysical Research, **115**, A02203 (2011).
2. Osman K.T. , Matthaeus H.M. , Greco A. ,Servidio S.,  
*Evidence for inhomogeneous heating in the solar wind*  
The Astrophysical Journal Letters, **727**, L11 (2011).
3. Romé M., Lepreti F.,  
*Turbulence and coherent structures in non-neutral plasmas*  
The European Physical Journal Plus, **126**, 38-1 (2011).
4. Valentini F., Califano F., Perrone D., Pegoraro F., Veltri P.,  
*New ion-wave path in the energy cascade*  
Physical Review Letters, **106**, 165002 (2011).
5. Perri S., Zimbardo G., Greco A.,  
*On the energization of protons interacting with 3-D time-dependent electromagnetic fields in the Earth's magnetotail*  
Journal of Geophysical Research , **116**, A05221 (2011).
6. Perrone D., Nigro G., Veltri P.,  
*A shell model turbulent dinamo*  
The Astrophysical Journal, **735**, 73 (2011).
7. Carbone F., Vecchio A., Sorriso-Valvo L.,  
*Spatio-temporal dynamics, patterns formation and turbulence in complex fluids due to electrohydrodynamics instabilities.*  
European Physical Journal E , **34**, 75 (2011).
8. Valentini F., Perrone D., Veltri P.,  
*Short-wavelength electrostatic fluctuations in the solar wind*  
The Astrophysical Journal, **739**, 51 (2011).
9. Servidio, S., Greco A., Matthaeus W. H., Osman K. T., Dmitruk P.,  
*Statistical association of discontinuities and reconnection in magnetohydrodynamic turbulence*  
Journal of Geophysical Research, **116**, A09102-1 (2011).
10. Valentini F., Califano F., Perrone D., Pegoraro F., Veltri P.,  
*Excitation of nonlinear electrostatic waves with phase velocity close to the ion-thermal speed*  
Plasma Physics and Controlled Fusion , **53**, 105017 (2011).
11. Servidio S., Dmitruk P., Greco A., Wan M., Donato S., Cassak P. A., Shay M. A., Carbone V., Matthaeus W. H.,  
*Magnetic Reconnection as an Element of Turbulence*  
Nonlinear Processes in Geophysics , **18**, 675 (2011).
12. Perrone D., Valentini F., Veltri P.,  
*The role of alpha particles in the evolution of the solar-wind turbulence towards short scales*  
The Astrophysical Journal, **741**, 43 (2011).
13. Abramenko V., Carbone V., Yurchyshyn V., Goode P., Stein R., Lepreti F., Capparelli V., Vecchio A.,  
*Turbulent Diffusion in the Photosphere as Derived from Photospheric Bright Point Motion*  
The Astrophysical Journal, **743**, 133 (2011).
14. Capparelli V., Vecchio A., Carbone V.,  
*Long-range persistence of temperature records induced by long-term climatic phenomena*



- Physical Review E, **84**, 046103 (2011).
15. Zimbardo G.,  
*Heavy ion reflection and heating by collisionless shocks in polar solar corona*  
Planetary and Space Science, **59**, 468 (2011).
  16. Trotta E.M., Zimbardo G.,  
*Quasi-ballistic and superdiffusive transport for impulsive solar particle events*  
Astronomy and Astrophysics, **530**, A130 (2011).
  17. Zelenyi L.M., Rybalko S.D., Artemyev A.V., Petrukovich A.A., Zimbardo G.,  
*Charged particle acceleration by intermittent electromagnetic turbulence*  
Geophysical Research Letters, **38**, L17110 (2011).
  18. Nisticò G., Patsourakos S., Bothmer V., Zimbardo G.,  
*Determination of temperature maps of EUV coronal hole jets*  
Advances in Space Research, **48**, 1490 (2011).
  19. Dmitruk P., Mininni P. D., Pouquet A., Servidio S., Matthaeus W. H.,  
*Emergence of very long time fluctuations and 1/f noise in ideal flows*  
Physical Review E, **83**, 066318 (2011).
  20. Parashar T. N., Servidio S., Shay M. A., Breech B., Matthaeus W. H.,  
*Effect of driving frequency on excitation of turbulence in a kinetic plasma*  
Physics of Plasmas, **18**, 092302 (2011).
  21. Servidio S., Carbone V., Dmitruk P., Matthaeus W. H.,  
*Time decorrelation in isotropic magnetohydrodynamic turbulence*  
Europhysics Letters, **96**, 55003 (2011).
  22. Greco A., Servidio S., Matthaeus W. H., Dmitruk P.,  
*Emergence of intermittent structures and reconnection in MHD turbulence*  
Advances in Plasma Astrophysics, **274** (2011).
  23. Nigro G., Veltri P.,  
*A Study of the Dynamo Transition in a Self-consistent Nonlinear Dynamo Mode*  
The Astrophysical Journal Letters, **740**, L37 (2011).
  24. Onofri M., Malara F., Veltri P.,  
*Role of anisotropic thermal conductivity in the reversed-field pinch dynamics*  
Physics of Plasmas, **18**, 052502 (2011).
  25. Zharkova V. V., Arzner K., Benz A. O., Browning P., Dauphin C., Emslie A. G., Fletcher L., Kontar E. P.,  
Mann G., Onofri M., Petrosian V., Turkmani R., Vilmer N., Vlahos L.,  
*Recent Advances in Understanding Particle Acceleration Processes in Solar Flares*  
Space Science Reviews, **159**, 357 (2011).
  26. Onofri M.,  
*Single-helicity states in compressible magnetohydrodynamics simulations of the reversed-field pinch with nonuniform resistivity*  
Nuclear Fusion **51**, 121003 (2011).

#### **A.1.2 Publications on international journals accepted in 2011**

1. Onofri M., Vecchio A., De Masi G., Veltri P.,  
*Propagation of gravity waves in a convective layer*  
to appear on The Astrophysical Journal.
2. Servidio S., Valentini F., Califano F., Veltri P.,  
*Local Kinetic Effects in Two-Dimensional Plasma Turbulence*  
to appear on Physical Review Letters.

3. Wan M., Oughton S. , Servidio S., Matthaeus W. H.,  
*von Kármán self-preservation hypothesis for magnetohydrodynamic turbulence and its consequences for universality*  
to appear on Journal of Fluid Mechanics
4. Greco A., Matthaeus W. H., D'Amicis R., Servidio S., Dmitruk P.,  
*Evidence for Nonlinear Development of Magnetohydrodynamic Scale Intermittency in the Inner Heliosphere*  
to appear on The Astrophysical Journal
5. Matthaeus W. H., Servidio S., Dmitruk P., Carbone V., Oughton S., Wan M., Osman K. T.,  
*Local anisotropy, higher order statistics, and turbulence spectra*  
to appear on The Astrophysical Journal.
6. Matthaeus W. H., Montgomery D. C., Wan M., Servidio S.,  
*A review of relaxation and structure in some turbulent plasmas: magnetohydrodynamics and related models*  
to appear on Journal of Turbulence.

## **B PUBLICATIONS ON CONFERENCE PROCEEDINGS**

### **B.1 Publications on international conference proceedings in 2011**

1. Matthaeus W. H., Montgomery D. C., Wan M., Servidio S.,  
*A review of relaxation and structure in some turbulent plasmas: magnetohydrodynamics and related models*  
Proceedings of the Conference “Turbulence Colloquium Marseille 2011”, Marseille, France (2011).
2. Nigro, G., Perrone, D., Veltri, P.,  
*A shell model for turbulent dynamos*  
Proceedings of the International Astronomical Union, IAU Symposium, vol. 274 , A. Bonanno, E. de Gouveia dal Pino & A. Kosovichev Eds., p. 159 (2011).
3. Perrone D., Valentini F., Veltri P.,  
*Hybrid Vlasov simulations for alpha particles heating in the solar wind*  
In “Advances in Plasma Astrophysics”, Proceedings IAU symposium 274, A. Bonanno, E. de Gouveia Dal Pino, A. G. Kosovichev Eds., IAU, p. 168 (2011).
4. Greco A., Servidio S. , Matthaeus W. H., Dmitruk P.,  
*Emergence of intermittent structures and reconnection in MHD turbulence*  
In “Advances in Plasma Astrophysics”, A. Bonanno, E. de Gouveia dal Pino, A. G. Kosovichev Eds., Cambridge University Press (2011).
5. Trotta E.M., Zimbardo G.,  
*Superdiffusive and ballistic propagation of protons in solar energetic particle events*  
Advances in Plasma Astrophysics, Proceedings of the International Astronomical Union, , A. Bonanno, E. de Gouveia Dal Pino, A. G. Kosovichev Eds.IAU, p. 198 (2011).
6. Vecchio A., Laurenza M., Meduri D., Carbone V., Storini M.,  
*Spatio-temporal variability of the photospheric magnetic field*  
In “Advances in Plasma Astrophysics” IAU Symposium No. 274, , A. Bonanno, E. de Gouveia Dal Pino, A. G. Kosovichev Eds., IAU, p. 204 (2011).

## **C INVITED PRESENTATIONS**

### **C1. Invited presentations at international conferences in 2011**

1. Califano F., Valentini F., Veltri P., Perrone D. ,  
*Turbulence transition across the ion cyclotron frequency: a Vlasov approach*  
478th Heraeus Seminar, Fusion and Astrophysical plasmas, Bad Honnef, Germany , April 18-20, 2011.
2. Greco A., Servidio S., Matthaeus W. H., Dmitruk P., Osman K.,  
*Statistical association of intermittent current sheets and reconnection in MHD turbulence*

- International Astrophysics Forum - Frontiers in Space Environment Research, Alpbach, Austria, June 20-24, 2011.
3. Malara F.,  
*Formation of discontinuities in the inhomogeneous magnetic field of a coronal hole*  
Arcetri 2011 Workshop on Plasma Astrophysics, Arcetri, Florence, Italy, October 17-21, 2011.
  4. Valentini F.,  
*Kinetic simulations in space plasmas*  
Plasma in Astrophysics and in the laboratory (PAL2) , Torino, Italy, November 23-24, 2011.
  5. Zimbardo G., Perri S. ,  
*Superdiffusive Transport at Shocks in Space Plasmas*  
IX COLAGE, Latin American Congress of Space Geophysics , Puntarenas, Costa Rica, April 4-10, 2011.
  6. Zimbardo G., Perri S., Pommois P., Veltri P. ,  
*Particle Transport in the Heliosphere*  
Advanced School of Space Environment (ASSE), IX Latin American Congress of Space Geophysics,  
Puntarenas, Costa Rica, April 4-10, 2011.
  7. Zimbardo G., Perri S.,  
*Superdiffusive transport at shocks in space plasmas*  
International Astrophysics Forum 2011, Frontiers in Space Environment Research, Alpbach, Austria, June 20-24, 2011.
  8. Perri S., Greco A., Zimbardo G.,  
*Stochastic acceleration of protons in the Earth's magnetotail current sheet: numerical studies*  
European Geosciences Union General Assembly 2011, Wien, Austria, April 3-8, 2011.
  9. Perri S., Greco A., Zimbardo G.,  
*Stochastic acceleration of protons in the Earth's magnetotail current sheet: numerical studies*  
XXX URSI GASS - International Union of Radio Science , Istanbul, Turkey, August 13-20, 2011.

## **D PRESENTATIONS AT CONFERENCES**

### **D1. Presentations at international conferences in 2011**

1. Valentini F., Califano F., Perrone D., Pegoraro F., Veltri P.,  
*Electrostatic fluctuations at short scales in the solar-wind turbulent cascade.*  
Vlasov-Maxwell kinetics: theory, simulations and observations in space plasmas, Wien, Austria, March 29 – April 1, 2011.
2. Perrone D., Valentini F., Veltri P.,  
*Nonlinear study of solar wind alpha particles heating through hybrid Vlasov numerical simulations*  
Vlasov-Maxwell kinetics: theory, simulations and observations in space plasmas, Wien, Austria, March 29 – April 1, 2011.
3. Sorriso-Valvo L., Carbone F., Strangi G.,  
*Anisotropy of spatio-temporal decorrelation in electrohydrodynamic turbulence*  
Liquid Matter Conference 2011, Wien, Austria, September 5-10, 2011.
4. Ciuchi F., Sorriso-Valvo L., Mazzulla A., Redondo J.M.,  
*Fractal aggregates evolution of methyl red in liquid crystal*  
Liquid Matter Conference , Wien, Austria, September 5-10, 2011.
5. Meduri D., Wicht J., Sorriso-Valvo L. and Carbone V.,  
*A Statistical Analysis of Reversal Sequences: Geomagnetic Field and Numerical Dynamo Models*  
European Planetary Science Congress , Nantes, France, October 2-7, 2011.
6. Carbone F., Vecchio A. and Sorriso-Valvo L.,  
*Spatio-temporal dynamics, patterns formation and turbulence in complex fluids due to electrohydrodynamics*

- instabilities  
Liquid Matter Conference , Wien, Austria, September 5-10, 2011.
7. Ciuchi F., Sorriso-Valvo L., Mazzulla A., Redondo J.M.,  
*Fractal aggregates evolution of red methyl in liquid crystal*  
Aggregation and Dynamic Arrest in Colloidal Systems , Rome, Italy, May 23-24, 2011.
  8. Marino R., Sorriso-Valvo L., Carbone V., Bruno R., Veltri P.,  
*The magnetohydrodynamic turbulent cascade in polar solar wind: the role of local dynamic alignment*  
EGU 2011, Wien, Austria, April 3-8, 2011.
  9. Zimbardo G., Greco A., Sorriso-Valvo L., Perri S., Voeroes Z., Aburjania G., Chargazia K., and Alexandrova O.,  
*Magnetic turbulence in the magnetospheric environment: highlights from multi-spacecraft missions*  
EGU 2011, Wien, Austria, April 3-8, 2011.
  10. Sorriso-Valvo L., Yordanova E., Carbone V. and Perri S.,  
*Multipoint measurement of solar wind turbulence anisotropy by Cluster*  
EGU 2011, Wien, Austria, April 3-8, 2011.
  11. Valentini F., Perrone F., Veltri P.,  
*Electrostatic fluctuations at short scales in the solar wind: Vlasov simulations*  
Arcetri 2011 Workshop on Plasma Astrophysics, Arcetri, Florence, Italy, October 17-21, 2011.
  12. Valentini F., Perrone D., Veltri P., Califano F., Pegoraro F.,  
*A new branch of electrostatic fluctuations: the ion-bulk waves*  
53<sup>rd</sup> annual meeting of the American Physical Society, Division of Plasma Physics, Salt Lake City, USA, November 14-18, 2011.
  13. Greco A., D'Amicis R., Matthaeus W. H., Servidio S., Dmitruk P.,  
*Evidence for development of intermittent structures in the inner heliosphere.*  
Arcetri 2011 Workshop on Plasma Astrophysics, Arcetri, Florence, Italy, October 17-21, 2011.
  14. Nigro G.,  
*A Shell Model for Turbulent Magnetic Dynamo*  
"RädlerFest: Alpha Effect and Beyond" , Stockholm, Sweden, February 14-18, 2011.
  15. Nigro G., Veltri P., Carbone V.,  
*Self-consistent Nonlinear Dynamo Mode*  
Arcetri 2011 Workshop on Plasma Astrophysics, Arcetri, Florence, Italy, October 17-21, 2011.
  16. Nigro G., Veltri P.,  
*Study on the Dynamo Transition in a Self-consistent Nonlinear Dynamo Model*  
EGU General Assembly, Wien, Austria, April 3-8, 2011.
  17. Onofri M.,  
*Single-Helicity states in compressible magnetohydrodynamics simulations of the reversed-field pinch with anisotropic thermal conductivity*  
14th European Fusion Theory Conference, Frascati, Italy, September 26-29, 2011.
  18. Onofri M.,  
*MHD simulations of the RFP with anisotropic thermal conductivity*  
15th International RFP Workshop, Madison, USA, October, 10-12, 2011.
  19. Onofri M.,  
*Compressible MHD simulations of the reversed-field pinch*  
PAL2 Workshop, Torino, Italy, November, 23-24, 2011.
  20. Servidio S.,  
Numerical experiments of magnetic reconnection in two-dimensional turbulence

Astronom 2011, the 6th Annual International Conference on Numerical Modeling of Space Plasma Flows in Valencia, Spain, 13-17 June, 2011.

21. Servidio S.,  
Local kinetic effects in two-dimensional plasma turbulence  
Arcetri 2011 Workshop on Plasma Astrophysics, Arcetri, Florence, Italy, October 17-21, 2011.
22. Servidio S.,  
*Magnetic reconnection in 2D simulations of turbulence*  
PAL2 Workshop, Torino, Italy, November 23-24, 2011.
23. Donato, S., Servidio, S., Dmitruk, P., Carbone, V., Shay, M. A., Matthaeus, W. H.,  
*Influence of Hall effect on reconnection in turbulence*  
American Geophysical Union, Fall Meeting 2011, San Francisco, USA, 2011.
24. Servidio, S., Greco, A., Matthaeus, W. H., Osman, K., Dmitruk, P.,  
*Statistical association of discontinuities and reconnection in magnetohydrodynamic turbulence*  
American Geophysical Union, Fall Meeting 2011, San Francisco, USA, 2011.
25. Greco, A., Matthaeus, W. H., D'Amicis, R., Dmitruk, P., Servidio, S.,  
*Evidence for Nonlinear Development of MHD scale Intermittency in the Inner Heliosphere*  
American Geophysical Union, Fall Meeting 2011, San Francisco, USA, 2011.
26. Matthaeus, W. H., Greco, A., Servidio, S., Wan, M., Osman, K., Ruffolo, D. J.,  
*The flux tube paradigm and its role in MHD turbulence in the solar atmosphere*  
American Geophysical Union, Fall Meeting 2011, San Francisco, USA, 2011.
27. Osman, K., Matthaeus, W. H., Wan, M., Greco, A., Servidio, S., Dmitruk, P.,  
*Statistical Analysis of Solar Wind Discontinuities: Inhomogeneous Heating, Intermittency, and Non-Gaussian Statistics*  
American Geophysical Union, Fall Meeting 2011, San Francisco, USA, 2011.
28. Servidio S., Wan M., Matthaeus W. H., Carbone V.,  
*Local relaxation and maximum entropy states in two-dimensional decaying turbulence*  
American Physical Society, 64th Annual Meeting of the APS Division of Fluid Dynamics, USA, November 20-22, 2011
29. Wan M., Oughton, S. Servidio S., Matthaeus W. H.,  
*On the accurate simulation of magnetohydrodynamic turbulence and magnetic reconnection*  
American Physical Society, 64th Annual Meeting of the APS Division of Fluid Dynamics, USA, November 20-22, 2011

## 2. BIOMEDICAL PHYSICS

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I. Nicotera (*University of Calabria, Chemistry Department*)

### Research subjects:

1. Dosimetry with new EPR-sensitive materials
2. Study of radiation effects in biomolecules

### Introduction

Technological developments in the field of Radiotherapy and Radioimaging push the research in physical dosimetry towards the study and the design of both new methodologies and new materials. Innovative radiotherapeutic methods have deeply affected the treatment of tumors located near critical organs, wrapped around a healthy anatomic structure, concave, or strongly irregular in shape. The dose delivery to the patient is improved by conforming the therapeutic radiation beam to the shape of the tumor. This allows a higher dose of radiation to be delivered to the tumor with respect to the surrounding normal tissues as compared with conventional techniques, for the purpose of achieving a better tumor control, with reduced toxicity of the radiation. However, new radiotherapeutic methods place significant demands on radiation dosimetry. Tighter treatment margins are necessary between the target tissue and the high-dose delivery, because of the strong field gradients which are present over the irradiated volume. Besides the accurate positioning of the patient, obtained by specialized Computer Tomography scanners and planning software, measuring the dose with the appropriate dosimeter system becomes a particularly significant step in order to effectively preserve normal tissues, avoiding marginal tumor recurrence, and, by avoiding critical organs, allow an overall better quality of life to the treated patient.

### 2.1 DOSIMETRY WITH NOVEL EPR-SENSITIVE MATERIALS

#### *Low-dose preclinical applications of EPR in radiotherapy*

The study of the radio-induced radicals in newly developed materials showing a higher sensitivity at low doses (below 10 Gy) expands the applicability of EPR-dosimetry to forefront radiotherapeutic methods. By a proper choice of the EPR-sensitive substance, very small EPR dosimeters can be produced, and the effective Z can be modulated from the average bodily value to those of its different tissue constituents. As a consequence, the perturbation induced by the dosimeter in the dose measurement can be very small, and accurate dose determination becomes possible in the case of dose administration with both special radiotherapeutic techniques and small fractionate-dose conventional radiotherapy. Recently, sugars, dithionates and formates have been studied as possible low-dose EPR materials. All of them show a higher sensitivity with respect to alanine, the EPR standard material. Interestingly, the latter materials can be modified by inclusion of paramagnetic species or isotope substitution in order to further increase low dose performances.

Fig. 1 shows the calibration curves obtained at doses in the therapeutic range by irradiation of Li-formate ( $\text{HCO}_2\text{Li}\cdot\text{H}_2\text{O}$ ) with photon beams at clinical energies (6 and 18 MeV).

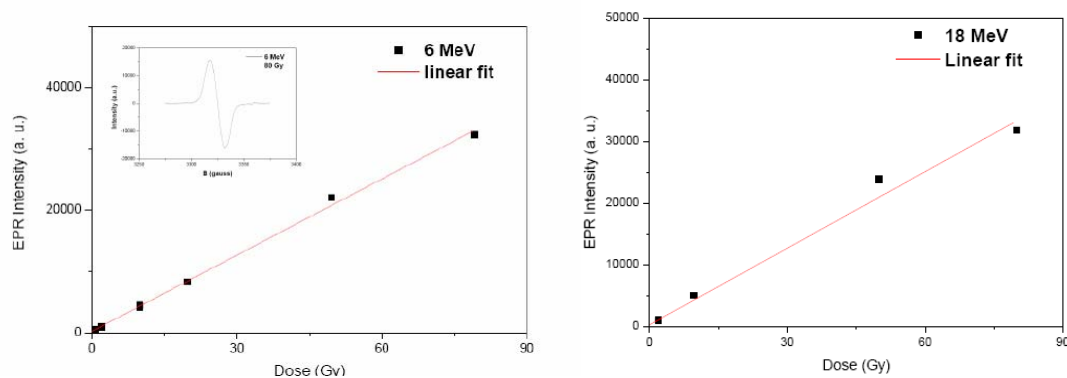


Figure 1. Li-formate calibration curves obtained for an irradiation energy of a) 6 MeV. Inset: EPR spectrum; b) 18 MeV. Also shown is the linear fit to the data. The calibration curves are obtained by plotting the peak-to-peak EPR intensity as a function of the irradiation dose.

The calibration curves are obtained by plotting the peak-to-peak EPR signal intensity of pure formate (shown in the inset) as a function of the irradiation dose. For the purpose of the measurement, we designed and realised a prototypal dosimeter which was used in a phantom for beam characterisation.

The clinical irradiations were performed in collaboration with Dr. G. Scalzo and Dr. I. Lovik of the Azienda Ospedaliera of Catanzaro. Preliminary checks of the dosimeter material and set-up (*A. Curcio, Tesi Triennale*) were performed with orthovoltage beams from a laboratory equipment (X-ray irradiator Faxitron 650X, typical energy used: 100 keV) at the Molecular Biophysics Laboratory in collaboration with Dr. Rita Guzzi.

## 2.2 STUDY OF RADIATION EFFECTS IN BIOMOLECULES

### *Synthesis and characterisation of modified formates*

Modified  $\text{HCO}_2\text{LiH}_2\text{O}$ , by inclusion of paramagnetic species (Ni, Zn, Cd), were prepared, irradiated and measured in the Molecular Biophysics Laboratory (*I. Bonetti, Tesi Magistrale, aa 2010/11*). The original study concerned the Zn and Cd doped samples, while Ni doping was performed for comparison purposes. Our preliminary results indicate larger sensitivities, with respect to alanine and the native material, for all studied samples. The EPR signal intensity depends on the metal atom concentration, in agreement with literature results on Ni-doped Li-formate. This allows, in principle, to miniaturise the dosimeter by using a reduced mass of the EPR sensitive material synthesised on purpose. Dosimetric tests with clinical beams are under way.

### *Dosimetric properties of HAp alginates*

We studied the time dependence of the EPR signal of Hydroxyapatite (HAp) alginates. Hydroxyapatite (HAp) is a synthetic, biocompatible material, radiosensitive with respect to electron paramagnetic resonance, presenting a relatively high effective Z value. Biologically, it corresponds to the mineral constituent of bone and teeth. In HAp alginates, nanograins of the radiosensitive species are embedded in a highly porous, low-Z value alginate matrix (see SEM picture in Fig.2).

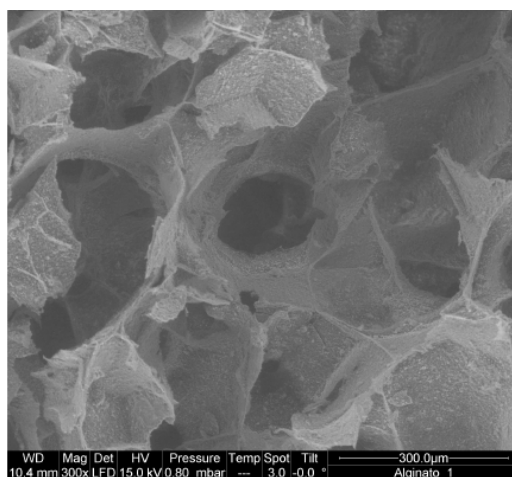


Figure 2 SEM picture of dry Hydroxyapatite alginate sample showing the interconnected pores (ESEM measurements, LICRYL–Liquid Crystal Laboratory, IPCF-CNR Cosenza).

The composite samples are synthesised by Dr. E. Marsich at the Life Science Department of the University of Trieste, where they are studied for their potential biotechnological applications for osteoimplants and artificial organs. We irradiated HAp alginate scaffolds, i.e. self-sustained samples, with the orthovoltage irradiator Faxitron 650X in a wide dose interval, including therapeutic dose values. We showed that the EPR signal is contributed by the radicals radioinduced in the inert grains located in the host alginate reticulate, by comparison with the signal from pure alginate and pure HAp powders. The intense EPR signal is time dependent within the first days after the irradiation. The presence of stable radicals suggests a possible dosimetric use as lung substitutes and phantoms.

### *Radioinduced modifications of carbohydrates*

Sugars are very sensitive EPR dosimetric materials and their effective Z value is very similar to the average value of the human body. They are used for retrospective dosimetry, which may be easily implemented in case of accidents or other un-programmed exposures, given the all-pervasive presence of sugars, in particular sucrose, in normal

households or in working environments (*F. Quaranta, Tesi Triennale, aa. 2010/11*). Sugars have also been suggested as economical, sensitive dosimeters for medical dosimetry. However, sugars are hygroscopic, and their complex, time-dependent multiple-radical spectrum may be affected by ambient humidity. We determined the time dependence of fructose and sucrose EPR spectra over a period of several months. In current laboratory conditions of temperature and humidity, a stable signal of fructose which is useful for dosimetry is achieved only after several months, while sucrose has developed a stable spectrum within 2 days from irradiation. The effect of humidity was studied by NMR analysis (PCSM-“M. Terenzi” Laboratory of the Chemistry Department -UNICAL) of caked sucrose samples obtained by keeping sucrose powders of different grain size under controlled humidity conditions (85%, 1 week in the presence of a saturated solution of KCl). Under these conditions water incorporation is according to the regimes B and C of caking, i.e., water is absorbed according to the funicular scheme (wetting, with permanent contact among particles) or capillary scheme (liquid bridges among particles, with no dissolution), respectively. Phase C is more abundant if the saccharose particles are smaller.

The  $^1\text{H}$ -NMR peak width, which is related to the  $T_2$  (spin-spin) relaxation time, is small (of the order of a ms), indicating that the water molecules are strongly interacting with the surface of the sucrose grains. Heating for one hour at 50 °C reduces the signal, owing to evaporation of the weakly bound water molecules.

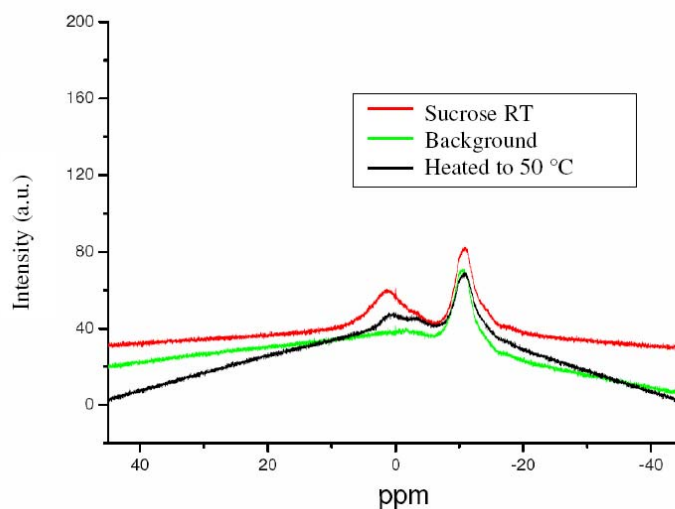


Figure 3. NMR proton spectra (90-Fid sequence) of caked saccharose. A single, weak  $^1\text{H}$ -NMR peak is observed (FWHM = 1 KHz).



## **B PUBLICATIONS ON CONFERENCE PROCEEDINGS**

1. Anna Santaniello, Ingunn Løvik, Rita Guzzi, Angelica Rania, Luigi Sportelli, Cesare Scalzo and Giuseppe Scalzo, *Preliminary study of an EPR clinical dosimeter based on L-i formate*  
VII National Congress of the Italian Association of Medical Physicists (AIFM), 13-16 September 2011, Squillace (CZ)-Italy.

## **D PRESENTATIONS AT CONFERENCES**

### **D. 2 Presentations at national conferences in 2011**

1. Anna Santaniello, Ingunn Løvik, Rita Guzzi, Angelica Rania, Luigi Sportelli, Cesare Scalzo and Giuseppe Scalzo, *Preliminary study of an EPR clinical dosimeter based on Li-formate*  
Oral presentation, VII National Congress of the Italian Association of Medical Physicists (AIFM), 13-16 September 2011, Squillace (CZ) Italy.
2. Anna Santaniello, Annamaria Giorno, Antonio Vecchio and Vincenzo Carbone, *Proper Orthogonal Decomposition as a diagnostic tool in Cardiology*  
Poster presentation, VII National Congress of the Italian Association of Medical Physicists (AIFM), 13-16 September 2011, Squillace (CZ)-Italy.
3. Anna Santaniello, Angelo Curcio, Rita Guzzi, Roberto Siciliano and Luigi Sportelli, *Preliminary characterisation of a commercial X-ray irradiator by means of EPR dosimetry*  
Poster presentation, VII National Congress of the Italian Association of Medical Physicists (AIFM), 13-16 September 2011, Squillace (CZ)-Italy.

### 3. CONDENSED MATTER PHYSICS

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Ernesto Pelaez (*Instituto de Quimica, Universidad de la Habana, Cuba*)

The research activity of the group is oriented in six closely related directions, which are briefly described in the following sections:

- 3.1 Surface Nanoscience
- 3.2 Ion induced and electron induced excitations in Graphene/substrate systems and Carbon nanotubes
- 3.3 Photon-matter interaction: electronic properties of graphene and related materials
- 3.4 Quantum coherence and correlations in condensed matter systems
- 3.5 Ion interaction with nanostructures and solids
- 3.6 Physics education

### 3.1 SURFACE NANOSCIENCE

Understanding the interaction of epitaxial monolayer graphite (MG) grown on transition metal (TM) with the substrate is an important step from both fundamental and technological point of view. Recently, we address our research on the fabrication and study of graphene over-layers epitaxially grown on metallic surfaces and intercalated with alkali atoms, in order to develop a fundamental understanding of the graphene-substrate interaction. We investigate electronic structure of the MG/metal system by surface spectroscopic techniques based on different probes: Auger electron spectroscopy (AES), high-resolution (HR) electron energy loss spectroscopy (EELS) and photoelectron spectroscopies (XPS, UPS).

Angle resolved (AR) EELS is mainly used to obtain information about the valence band structure and the momentum-space-dependence of collective excitations in graphene foils grown on metallic substrates. Electron emission from well ordered thin films, excited by photons or monochromatized electrons, follows the conservation laws of energy and momentum parallel to the surface. This means that the parallel component of the wave vector of either the valence electrons or the excited plasmons can be obtained together with the energy. In particular, we are focusing on two-dimensional (2D) plasmons, whose charge fluctuations are strongly localized at a monolayer. Graphene is a significant testing ground of the microscopic dielectric theory of 2D systems, being its electronic states confined in one atomic-layer thickness. For this reason, it has been recently indicated as a promising material also for nanoplasmonics, an emerging field that deals with the employment of collective excitations for developing new devices. Plasmonic components can be used to improve the resolution of microscopes, the sensitivity of chemical detectors, the efficiency of Light-Emitting Diodes (LEDs).

One of the outstanding features of a 2D free electron gas is the square-root dependence of plasmon energy on the parallel wave vector, in contrast with the parabolic dispersion law typical of 3D systems. The 2D collective electron excitation modes, determined by charge fluctuations strongly localized at a monolayer, have been discussed theoretically for a long time. However, few experimental data have been reported and no clear experimental evidence of the anomalous dispersion was found, likely because of the weak localization of electronic states of the atomic over-layers under study. The electronic states of MG/metal systems are instead characterized by a very strong localization at the over-layer plane, due to the large anisotropic chemical C-C bond of graphite, thus leading to 2D electronic states confined in one atomic-layer thickness.

We found that the influence of the substrate induces a change in the charge distribution, and consequently in the dispersion on the parallel wave vector, and assigned another branch at energies above 6.0 eV to the longitudinal 2D plasmon related to interband transitions involving interface states. The hybridization of  $\pi$  orbital of MG with  $d$  bands of the substrate induces a partial population of conduction band states near the Fermi level, leading to the observed 2D plasmon at lower energy. Therefore, the strength of the interaction between MG and the underlying substrate can be determined by monitoring the Fermi surface in the graphene over-layers.

We expect, in fact, that the intensity of this intraband electronic excitation and the value of its energy strongly depends on the number of charge carriers occupying hybrid electronic states. On the other hand, the localization of these states in one atomic layer give a 2D character to the plasmon, allowing us to add more experimental evidence for the dispersion relations. It is worth noting that this collective excitation cannot occur in the zero-gap free-standing graphene, unless either temperature is non-zero or graphene is driven away from the charge neutrality point by doping or gating. The MG-substrate coupling is responsible of the onset of this collective excitation; nevertheless, the presence of the substrate does not alter the plasmon 2D nature, and tunable hybridization between electronic states of graphene and the metal surface can be exploited to modify the plasmon behaviour, as it depends on the charge carriers distribution. For the purpose of recovering the intriguing electronic properties of freestanding graphene at a solid surface, the way of producing a single epitaxial graphene layer and decoupling it from substrate has been studied in recent years. It has been observed that the intercalation of metals underneath a graphite monolayer results in a weakening of the interaction between graphene ad-layer and the substrate. As a consequence, a reversal of the energetic shift of the graphite derived electronic states in the valence band and of the phonon modes toward the positions

characteristic for pristine graphite was indeed measured. In this respect, intercalation of foreign atoms into the graphene/metal interface offers an appealing possibility to control the degree of hybridization between the substrate and C-2p<sub>z</sub> orbitals. In our recent investigations we have studied the process of intercalation of Cs atoms underneath a graphite monolayer formed on Ni(111). Angle-resolved electron-energy-loss spectroscopy has been used to compare the momentum-space-dependent behaviour of  $\pi$  plasmon on epitaxial graphene on Ni(111) and on the same system intercalated by atoms of cesium. The dispersion curves were found to be significantly different: a square-root behavior of the plasmon mode is observed in epitaxial graphene, allowing us to conclude that the fluctuating charge density is strictly two-dimensional; a linear  $\pi$  plasmon dispersion is observed in the same system intercalated by Cs atoms; the combine between the linearity of dispersion curve with the  $\pi$  band linearity at Dirac points shows how alkali metal atoms makes graphene to be quasi-free with the recovery of the typical Dirac cones observed in free standing flakes. Therefore, we consider the  $\pi$  plasmon dispersion as a fingerprint for the degree of isolation, indeed the strictly linear dispersion of this mode is only visible in isolated graphene sheet where the recovery of Dirac cones occurs.

Previous works exploited the modifications of the electronic structure of the valence band and of the phonon spectra caused by different metal atoms intercalation. They demonstrated how this intercalation takes the system closer to ideal freestanding graphene, with the “stiffening” of the phonon modes, and with the recovery of the  $\pi$  band linearity at Dirac points. In relation to electronic properties, for the first time we also demonstrated that graphene collective excitations can be tailored by intercalation of alkali metal atoms. However, perspective of graphene for nanoplasmonics are largely unexplored since plasmon modes of graphene flakes have not been addressed so far. As our results indicate, a great amount of control over graphene plasmon properties makes it a very promising material for applications.

### **3.2 ION INDUCED AND ELECTRON INDUCED EXCITATIONS IN GRAPHENE/SUBSTRATE SYSTEMS AND CARBON NANOTUBES**

The 2011 research activity was devoted to ab-initio modeling of carbon based nanostructures, in free standing forms and deposited on metal surfaces, combined with theoretical and experimental studies of ion induced and electron induced excitations.

As a preliminary phase, existing density functional theory (DFT) approaches were tested on free standing Graphene, (n,n) and (n,0) Carbon Nanotubes (CNTs), Graphene Slabs and Graphene deposited on Ni(111) substrates. More specifically, both atomistic and periodic DFT computations were performed using LDA, GGA, and DFT+U functionals, with plane-wave and tight-binding basis sets. The DFT+U hybrid approach, in which an additional energy term needs to be added to the LDA or GGA exchange-correlation energy, was considered to improve the ground state description of the Nickel slab. In finite size calculations, clusters of 500-1000 atoms were used to simulate the geometric structure of graphene, as well as (10,10) and (17,0) CNTs. In periodic calculations, super-cells of 2-11 atoms were taken into account, with a Monkhorst-Pack grid of the order of 2500-5000 k points in the first Brillouin zone, to simulate Graphene, Graphite, and Graphene/Ni(111) systems. A vacuum of 10-20 Angstroms was adopted to separate the slabs. Once the ground state properties were determined, calculations of deep-hole excited states were performed using ionized atomic pseudo potentials. The one-electron orbitals, entering both the ground and the excited states of the systems, were used to calculate the energy distributions of electron ejected from the samples, via X-ray or Auger processes. Linear time-dependent DFT methods were applied to the determination of the dielectric response of the systems, including the energy loss spectra.

Concerning the experimental side, secondary electron spectroscopy was used to probe the excited states of graphene adsorbed on a Ni(111) surface. We measured energy distribution and yields of electrons emitted from graphene adsorbed on a Ni(111) surface under the impact of 200-1200 eV electrons. The adsorption of graphene results in significant changes of the spectra of emitted electrons but not of the total emission yields. The electronic structure of the graphitic over-layer affect the energy distribution of emitted electrons, determining the final states of excited electrons transported by collision cascade from the bulk of the substrate. A fine structure directly related to the empty bands above the vacuum level of the sample was resolved in the spectra excited by electrons. A high energy feature was identified in Ion-induced spectra that is consistent with electron promotion from valence to conduction band states, from which electrons emerge into vacuum. The graphene/Ni(111) system was also investigated by angle-resolved electron-energy-loss spectroscopy. The interface pi plasmon, related to interband transitions involving hybridized states at the K point of the hexagonal Brillouin zone, was measured at different scattering geometries. The resulting dispersion curve were shown to exhibit a square root behavior, indicating the 2D character of the interface collective excitation.

### **3.3 PHOTON-MATTER INTERACTION: ELECTRONIC PROPERTIES OF GRAPHENE AND RELATED MATERIALS**

This research line concerns with the study of the electronic properties of graphene and related materials by means of synchrotron radiation. Specifically, graphene sheets prepared by the exfoliation method and epitaxially grown on transition metals have been studied through the photoemission and photoabsorption process induced by a synchrotron

light source.

In collaboration with the *Istituto di Struttura della Materia-CNR* of Trieste, we have performed our experiments at the beam line *VUV Photoemission* of the Synchrotron *Elettra*, by means of Angle-Resolved Photoemission Spectroscopy (ARPES). This technique has probably contributed more than any other experimental tool to verify the notion of the electronic bands and of some other fundamental concepts, like crystal momentum, Umklapp processes or the Brillouin zone. Thanks to the development of experimental equipments, nowadays ARPES can explore subtle many-body effects, which challenge our understanding of band theory. A photoemission spectrum is in fact directly related to the one particle spectral function  $A(k, \omega)$ , a fundamental theoretical quantity which contains exhaustive information on the excitation spectrum of a many body system, and therefore of the nature and strength of the interactions. In particular, if the experimental energy and momentum resolution are sufficiently high, ARPES can probe the fundamental quasiparticle states (or signal their absence), which determine the thermodynamic properties of a material. This method is ideal to investigate the conical dispersion of the  $\pi$  band of graphene at the K point of the Brillouin zone.

The low-energy excitations in graphene depend to a surprising extent on the interaction strength with the metal that serves as support. By varying the support itself or by intercalation of foreign atoms it is possible, through electron hybridization and structural modifications, to tailor graphene electronic properties. Variable interaction strengths can thus provide an additional control over the properties of graphene and may open new fields of applications.

We have shown how the electron group velocity, chirality, and bandgaps can be tailored by periodic perturbing potential, doping, intercalation, and hybridization with the supporting substrate. Moreover, we have illustrated how the structural and electronic properties of epitaxial graphene are modified by the interaction with magnetic layers and self-assembled magnetic clusters.

### **3.4 QUANTUM COHERENCE AND CORRELATIONS IN CONDENSED MATTER SYSTEMS**

This research line is devoted to the theoretical investigation of the role of quantum coherence and correlations (entanglement and discord) in the quantum optical and condensed matter physics of mesoscopic systems. In 2011, the research activity has been developed along to two main directions: 1) spin systems and 2) Quantum correlations suppression and decoherence.

#### **3.4.1 Spin systems**

We studied the dynamics of a chain of interacting quantum particles affected by individual or collective multi-mode environment, focusing on the role played by the environmental quantum correlations over the evolution of the chain. The presence of correlations in the state of the environmental system magnifies the non-markovian nature of the chain's dynamics, giving rise to structures in figures of merit such as entanglement and purity that are not observed under a separable multi-mode environment. This analysis can be relevant to problems tackling the open-system dynamics of biological complexes. Furthermore, we investigated the transfer of quantum correlations across the chain and compared the transport of quantum discord with that of entanglement, addressing various operating regimes. Discord turns out to be better transported for a wide range of working configurations and initial conditions of the system. We related this behaviour to the efficiency of propagation of a single excitation across the effective channel embodied by the chain.

#### **3.4.2 Quantum Correlation suppression and Decoherence**

We studied the dynamics of entanglement between two qubits coupled to independent reservoirs and between the two, initially disentangled, reservoirs. We also described the transfer of bipartite entanglement from the two-qubits to their respective reservoirs focusing on the case of two atoms inside two different leaky cavities with a specific attention to the role of the detuning. We also discussed a scheme to prepare the cavity fields

in a maximally entangled state, without direct interaction between the cavities, by exploiting the initial qubits entanglement.

### **3.5 ION-MATTER INTERACTION**

#### **3.5.1 Ion interaction with nanostructures**

We conducted a study on ion implantation and atom deposition on carbon nanostructures, by using several spectroscopy techniques. Interaction of atoms with carbon nanostructures actually holds an important role in scientific research because of its implications in advanced technological applications (nanoelectronics, nanolithography, photovoltaic ...). The interest in these intercalated compounds is due to changes in electronic and mechanical properties induced by the intercalates, which can lead to technological applications of the new materials. We employ the CEAES technique (Collisionally Excited Autoionization Electron Spectroscopy). This electron spectroscopy, induced by atomic collisional processes, allows us to monitor the amount of implanted ions by observing the change in intensity of such

atomic features as a function of the dose of projectile ions. Through this spectroscopy we are able to study changes of the sample local electrostatic potential (work function) by observing the spectral lines shift, since the kinetic energy of electrons emitted by atomic particles near the surface is strictly related to the electrostatic potential difference between the sample and the analyser. The full width at half maximum (FWHM) of observed lines can provide information about the homogeneity of the sample region beneath the decaying atoms. In fact the de-excitation should take place at a distance of 10 Å from the surface. The electrostatic potential seen by the emitted electron is thus an average over the (macroscopically very limited) underlying sample region, and the presence of impurities (for example, Na implanted atom) on the surface should inevitably cause a broadening of the spectral lines. On the other hand, if we compare to the techniques used, we observe a difference between implantation and evaporation. Our results show again that the implantation technique leads to a higher surface concentration of atoms, or, in the case of evaporation, the atom diffusion into the bulk is more probable.

We have observed how the properties of the carbon nanotubes (CNT) are strongly linked to the presence of impurities within the sample itself, for this purpose we have developed a new technique that allows purifying carbon nanotubes at relatively low temperature, through the absorption and subsequent desorption of alkali metals.

As well as create intercalate composites, we can grow nanocomposites with CNT. The doping of carbon nanotubes with organic and inorganic compounds (with formation of covalent and non-covalent bonds) can provide new properties and may lead to new applications. The covalent bonds with carbon nanotubes include mainly oxidation and formation of amide bonds, while non-covalent approaches utilize van der Waals interactions between functional compounds and CNT. Non-covalent approach has attracted more attention for the opportunity to grow nanocomposites with new properties while still preserving all the properties of the nanotubes. For example, the change of optical properties of CNT-based heterostructures assume particular importance to try improving the luminescence properties of carbon nanotubes in the visible range and open the possibility to use CNT in optoelectronics devices. Usually, to create uniform nanocomposites specialized technique are required; so we have growth nanocomposites of carbon nanotubes implementing a simple chemical mix method. The nanocomposites obtained were characterized by SEM, XPS, AES and luminescence spectroscopy. We observe that the heterostructures constituted by CNT and by doping elements (TiO<sub>2</sub>, LiF, ZnS, ...) form an uniform nanocomposite. The heterostructures observed are very different than that obtained by other techniques (for example evaporation). In the first one (chemical mix) the CNT is wrapped on doping elements without chemical bonds, showing changes in electronic and photoemission properties. While, with the evaporation, the elements diffuse in the bulk or shows two separated and superimposed films.

### 3.5.2 Radiation interaction with solids

Electrochromism is the property for which the color of a material changes reversibly in response to an externally applied potential. In the last years many efforts have been concentrated in developing electrochromic [EC] devices as EC windows, car mirrors, and display panels. In our work on radiation absorbance from EC devices, we have studied the visible range spectral features of viologen inserted into a polymer plasticized matrix of electrochromic films illustrated in previous works. We used ethyl viologen instead of other viologens, having longer chemical groups linked to nitrogen, because of its greater solubility into the plastic matrix. On the other hand, the methyl viologen has been excluded due to its well-known high toxicity. A suitable polymer matrix is the polyvinyl formale (PVF) plasticized with propylene carbonate (PC), a solvent with high dielectric constant and high boiling temperature. Useful film formulations fall in 30–40% PVF, 55–65% PC composition ranges. Taking into consideration the dielectric constant of PC, ranging from about 65 at room temperature, and that of the PVF, which is around 3, the average dielectric constant of the host matrix for viologen salts falls in the range 39–42, which is almost half of the water dielectric constant. So in this case, following the conclusions of Monk, no dimer formation of the monocation species, originated by the dication reduction, should occur. This idea is strongly supported by the fact that the blue color, observed in the operations of the electrochromic devices based on the previously discussed electrochromic film, never turns into violet. Another factor that should prevent dimer formation in our system is the reduced molecular diffusion, a very viscous plastic environment, should make very improbable the contact between different monomer monocations, at least during short operation times. Despite this simplification, the spectra of the reduced species may remain quite complex due to the presence of other mechanisms. First of all the formation of the neutral species V<sup>0</sup> must be taken into account. Then the possibility of complex formation between viologen species and oxygen, always endemically dissolved into the solvent, must also be considered. Concerning the second point, enough literature data support the importance of this mechanism: particularly relevant are the studies carried out by Ogawa et al. and Milosavljevic.

### 3.5.3 Diagnostic in cultural heritage

In the past the knowledge of ancient artifact took place almost exclusively through the art-historical approach, without any support from scientific investigation methodologies, allowing researchers a complete diagnosis of the object. Recently, scientific methods have been gradually asserting that allow us to go back to the age of archeological findings by a relative or absolute dating approach. The age of an artifact can be derived through the composition of the material of the object: for example, knowing the composition of a bronze or a ceramic we can trace back to their place

of manufacture and to the age of the finding itself. For this purpose, spectroscopic investigation techniques such as XPS, AES, luminescence etc. have been proven very useful. Moreover, this type of investigations also provide useful information for the planning of restoration interventions, since they allow to determine the composition of external agents that attacked the findings. In our laboratory, the composition of some bronze findings have been investigated, to detect the "diseases" of bronzes due to pollution and oxidation. The same spectroscopic techniques were also employed in the analysis of carousels from different sites in Calabria. The study of carousels was also accompanied by absolute dating methods such as ThermoLuminescence (TL) and Optically Stimulated Luminescence (OSL), which allowed to place temporally the analyzed carousels. In this regard, two measurement protocols were employed: SAR, Single Aliquot Regenerative-dose, and MAAD, Multiple Aliquot Additive Dose.

### **3.6 PHYSICS EDUCATION RESEARCH (PER)**

Laboratorial activities employing either cheap materials or high-tech low-cost devices (such as PC webcams and audio cards) are progressively recognized as a key topic for promoting the diffusion of hands-on activities in school physics laboratories. On the other hand, some conceptual knots concerning the graphical representation of magnetic fields are still under discussion in the international PER community, especially for the role they play in the comprehension of electromagnetic phenomena, including e.m. induction and Foucault dissipation. In this context, we have developed some some laboratorial learning paths for high school students, aiming to promote their skills regarding, among others, field-line representation of magnetic field. Developed learning paths have been tested in a high school network. Besides these didactical experimentations, some theoretical aspects have been investigated aiming to clarify some subtleties regarding macroscopic energy balance in the electromagnetic interactions, with particular regard to Foucault dissipation.

## A. PUBLICATIONS ON SCIENTIFIC JOURNALS

### A.1 Publications on international journals

#### A.1.1 Publications on international journals printed in 2011

1. M. Barberio, D. Barca, P. Barone, V. Pingitore, A. Bonanno, *Cathodo-luminescence from extrinsic impurities in bundles of carbon nanotubes: a possible role*, Journal of Nanoscience and Nanotechnology 11, 9196-9201 (2011).
2. A. Bonanno, G. Bozzo, M. Camarca and P. Sapia, *Using a PC and external media to quantitatively investigate electromagnetic induction*, Phys. Educ. 46 (2011) 385-394.
3. A. Bonanno, M. Camarca and P. Sapia, *Magnetic interactions and the method of images: a wealth of educational suggestions*, European Journal of Physics 32 (2011) 849-866.
4. A. Bonanno, G. Bozzo, M. Camarca and P. Sapia, *Foucault dissipation in a rolling cylinder: a webcam quantitative study*, European Journal of Physics 32 (2011) 419-429.
5. D. Pacilé, J. C. Meyer, A. Fraile Rodriguez, M. Papagno, C. Gomez-Navarro, R. S. Sundaram, M. Burghard, K. Kern, C. Carbone, and U. Kaiser, *Electronic properties and atomic structure of graphene oxide membranes*, Carbon 49, 966-972 (2011).
6. A. Sindona, M. Pisarra, P. Riccardi, G. Falcone, *Many-Body Effects in Auger Electron Emission from Finite-Length Carbon Nanotubes*, Nanoscience and Nanotechnology Letters, Volume 3, Number 6, November 2011, pp. 835-840(6).
7. A. Sindona, M. Pisarra, S. Maletta, M. Commisso, P. Riccardi, A. Bonanno, P. Barone, G. Falcone, *Role of Many Body Shake-Up in Core-Valence-Valence Electron Emission from Single Wall Carbon Nanotubes Source*, Journal of Nanoscience and Nanotechnology, Volume 11, Issue 10 Pages: 9143-9152, 2011
8. M. Pisarra, A. Cupolillo; L. S. Caputi, A. Sindona, P. Riccardi, *Secondary Electron Spectra of Graphene on Ni(111) Surface*, Journal of Nanoscience and Nanotechnology, Volume: 11 Issue: 10 Pages: 9256-9259, 2011
9. A. Sindona, M. Pisarra, S. Maletta, P. Riccardi, A. Cupolillo, G. Falcone, *Wave packet evolution of the valence state of a hyperthermal sodium ion impinging on a copper surface*, Nuclear Instruments and Methods in Physics Research, Section B - Beam Interactions with Materials and Atoms, Volume: 269 Issue: 9 Pages: 938-942, 2011
10. M. Pisarra, A. Sindona, P. Riccardi, *Molecular dynamics study of kinetic electron emission induced by slow sodium ions incident on gold surfaces*, Nuclear Instruments and Methods in Physics Research, Section B - Beam Interactions with Materials and Atoms, Volume: 269 Issue: 9 Pages: 981-984, 2011
11. T. J. G. Apollaro, C. Di Franco, F. Plastina and M. Paternostro, *Memory-keeping effects and forgetfulness in the dynamics of a qubit coupled to a spin chain*, Phys. Rev. A 83, 032103 (2011)  
Also selected by Virtual Journal of Quantum Information, Vol. 11, Issue 3, March 2011.
12. S. Campbell, T. J. G. Apollaro, C. Di Franco, L. Banchi, A. Cuccoli, R. Vaia, F. Plastina, and M. Paternostro, *Propagation of non-classical correlations across a quantum spin chain*, Phys. Rev. A 84, 052316 (2011).  
Also selected by Virtual Journal Nanoscale Science & Technology, Vol. 24, Issue 22, 28 November 2011.  
Also selected by Virtual Journal of Quantum Information, Vol. 11, Issue 11, November 2011.
13. S. Lorenzo, F. Plastina and M. Paternostro,



*The role of environmental correlations in the non-Markovian dynamics of a spin system*,  
 Phys. Rev. A 84, 032124 (2011).  
 Also selected by Virtual Journal of Biological Physics Research, Vol. 22, Issue 7, October 2011.  
 Also selected by Virtual Journal of Quantum Information, Vol. 11, Issue 10, October 2011

14. F. Plastina and S. Maniscalco,  
*Non-Markovian dynamics of system-reservoir entanglement*,  
 Int. J. Q. Info. 9, 1715-1726 (2011).

#### **A.1.2 Publications on international journals accepted in 2011**

1. M. Barberio, P. Barone, A. Bonanno, A. Oliva,  
*A new purification technique for single-walled carbon nanotubes by interaction with alkali and oxygen*,  
 Journal of Nanoscience and Nanotechnology. doi:10.1166/jnn.2012.4933.
2. C. Gattuso, D. Renzelli, P. Barone, V. Pingitore, A. Oliva,  
*S.A.R. and MAAD TL dating of "caroselli" from three sites in Calabria, south Italy*,  
 Mediterranean Archaeology & Archaeometry.
3. P. Barone, M. Barberio, A. Oliva and A. Bonanno,  
*Synthesis and characterization of carbon nanotubes wrapped on anatase microparticles*,  
 in Particle & Particle Systems Characterization doi:10.1002/ppsc.201200003.
4. M. Barberio, P. Barone, V. Pingitore and A. Bonanno,  
*Optical properties of TiO<sub>2</sub> anatase – Carbon Nanotubes composites studied by cathodoluminescence spectroscopy*,  
 Superlattice and Microstructure.
5. M. Barberio, P. Barone, R. Vasta, G. Manicò and F. Xu,  
*Formation of molecular nitrogen and diazene by electron irradiation of solid ammonia*,  
 Thin Solid Films. doi:10.1016/j.tsf.2012.03.112.
6. M. Barberio, P. Barone and A. Oliva,  
*Optical properties of ZnS – Carbon Nanotubes composites*,  
 Radiation Physics and Chemistry.
7. V. Pingitore, M. Barberio, P. Barone, A. Oliva,  
*Photoluminescence emission from Carbon Nanotubes based composites*,  
 Nanoscience and Nanotechnology Letters.
8. A. Bonanno, M. Camarca, P. Sapia,  
*The Casimir effect: A multimedia and hands-on integrated approach*,  
 International Journal on Hands-on Science.
9. M. Papagno, S. Rusponi, P. M. Sheverdyeva, S. Vlaic, M. Etzkorn, D. Pacilé, P. Moras, C. Carbone, and H. Brune,  
*Large Band Gap Opening between Graphene Dirac Cones Induced by Na Adsorption onto an Ir Superlattice*,  
 to appear on ACS Nano (2012).
10. D. Topwal, U. Manju, D. Pacilé, M. Papagno, D. Wortmann, G. Bihlmayer, S. Blugel and C. Carbone,  
*Quantum electron confinement in closely matched metals: Au films on Ag(111)*,  
 to appear on Phys. Rev. B (2012)
11. A. Cupolillo, N. Ligato, L.S. Caputi,  
*Two-dimensional character of the interface- $\pi$  plasmon in epitaxial graphene on Ni(111)*,  
 accepted by Carbon .
12. A. Sindona, M. Pisarra, P. Riccardi, G. Falcone,  
*Cluster and periodic density functional study of Auger Electron Emission from conducting Carbon Nanotubes*,  
 accepted by Journal of Nanoscience and Nanotechnology Letters.

13. M. Pisarra, P. Riccardi, A. Cupolillo, L.S. Caputi, A. Sindona,  
*Secondary electron spectroscopy of Graphene/Nickel(111)*,  
accepted by Journal of Nanoscience and Nanotechnology Letters.

### **A.1.3 Papers submitted for publication in 2011**

1. M. Barberio, P. Barone, V. Pingitore, A. Bonanno, F. Xu, A. Oliva,  
*Preparation of carbon nanotube/TiO<sub>2</sub> nano-composites film by an evaporation technique in UHV ambient*,  
Journal of Nanoscience and Nanotechnology
2. P. Barone, M. Barberio, V. Pingitore and A. Bonanno,  
*Transport properties of alkali-doped multi walled carbon nanotubes*,  
Journal of Nanoscience and Nanotechnology.
3. M. Barberio, P. Barone, V. Pingitore, F. Xu,  
*Luminescence Emission from silver – carbon nanotubes composites*,  
Journal of Physics and Chemistry of Solids.
4. M. Barberio, P. Barone, V. Pingitore, A. Bonanno,  
*UV luminescence emission from LiF<sup>+</sup> – Carbon Nanotubes composites*,  
Physica E.
5. M. Barberio, R. Vasta, P. Barone, G. Manicò and F. Xu,  
*Experimental and theoretical study on the ethane and acetylene formation from electron irradiation of methane ices*,  
SuperLattice and Microstructures.
6. A. Bonanno, M. Camarca and P. Sapia,  
*Reaching the equilibrium: The role of dissipation in analogous systems*,  
European Journal of Physics.
7. A. Cupolillo, N. Ligato, L.S. Caputi,  
*Low energy two- dimensional plasmon in epitaxial graphene on Ni(111)*,  
Plasmonics

## **B PUBLICATIONS ON CONFERENCE PROCEEDINGS**

### **B.1 Publications on international conference proceedings in 2011**

1. A. M. Barberio, P. Barone, V. Pingitore, A. Bonanno, F. Xu, A. Oliva,  
*Preparation of carbon nanotube/TiO<sub>2</sub> nano-composites film by an evaporation technique in UHV ambient*,  
5th International Meeting on Developments in Materials, Processes and Applications of Emerging Technologies (MPA-2011) 27-29 June 2011, Alvor (Portugal).
2. P. Barone, M. Barberio, V. Pingitore, A. Oliva,  
*Transport Properties of alkali-doped- multi wall carbon nanotubes mats*,  
6th International Conference on Surfaces, Coatings and Nano-Structured Materials (NANOSMAT) 17-20 October 2011, Crakow (Poland).
3. A. Bonanno, P. Sapia, Y.L.T. Ting,  
*Multi-media CLIL: Enhancing technology-enhanced learning*.  
Proceedings of: “International Conference of Education and New Learning Technologies – EDULEARN 2011”  
– Barcelona, Spain – 4-6/07/2011.

## **C BOOK CHAPTERS**

1. M. Camarca, A. Bonanno, P. Sapia,  
*Nascita e crisi del metodo scientifico*,  
in *Filosofia e Scienza*, a cura di R. Cirino e A. Givigliano. Aracne Editrice, Roma. (Accepted 2011).

## **D INVITED PRESENTATIONS**

### **D.1 Invited presentations at international conferences in 2011**

1. D. Pacilé,  
Near-edge X-ray absorption fine-structure investigation of free-standing graphene and graphene oxide membranes,  
EMRS Spring Meeting 2011 (May 10-12, 2011, Nice, France)
2. D. Pacilé,  
*Angle-resolved photoemission studies of epitaxial graphene grown on selected transition metals and interactions with chemical dopants*,  
Atom based Nanotechnology (January 19, 2011, Firenze, Italy)
3. F. Plastina,  
*Memory-keeping effects and forgetfulness in the dynamics of a qubit coupled to a spin chain*,  
IQISC2011, Vietri sul mare (SA) 19-4-2011.
1. A. Sindona,  
*Cluster and periodic density functional study of Auger Electron Emission from conducting Carbon Nanotubes*,  
NANOSCIENCE AND NANOTECHNOLOGY 2011, 19-23 Sep 2011, Frascati, ROMA

## **E PRESENTATIONS AT CONFERENCES**

### **E.1 Oral Presentations at international conferences in 2011**

1. A. Bonanno, G. Bozzo, M. Camarca, M. Michelini, P. Sapia,  
*“Free Ideas”: Results from an innovative project for teacher development in Calabria (Italy)*,  
International Research Group on Physics Teaching” 2011 Conference (GIREP 2011). University of Jyväskylä, Finland, 1 - 5 August 2011.
2. A. Bonanno, M. Camarca, P. Sapia,  
*The Casimir effect: A multimedia interactive tutorial*,  
*16th International Conference on Multimedia in Physics Teaching and Learning” – Ljubljana, Slovenia – 15-17/09/2011.*
3. A. Bonanno, P. Sapia, Y.L.T. Ting,  
*Multi-media CLIL: Enhancing technology-enhanced learning*,  
*International Conference of Education and New Learning Technologies – EDULEARN 2011” – Barcelona, Spain – 4-6/07/2011.*
4. F. Plastina,  
*Quantum information and excitation transfer in spin chains*,  
WESS2011, Lecce 20-10-2011.
5. P. Riccardi,  
*Electron emission in the interaction of slow ions and electrons with nanostructured surfaces*,  
Deutsche Physikalische Gesellschaft – DPG - 75th Annual Meeting of the DPG and DPG Spring Meeting-  
Dresden, 13th - 18th of March 2011.
6. M. Pisarra,  
*Electron Emission from Finite Size Cylindrical Carbon Nanotubes: An Atomistic View*,  
MPA 2011 Development in materials, processes and applications of emerging technologies Alvor, Portugal,  
27-29 June 2011
7. M. Pisarra,  
*Secondary Electron Emission from Graphene Adsorbed on Ni(111) Surfaces*,  
MPA 2011 Development in materials, processes and applications of emerging technologies Alvor, Portugal,  
27-29 June 2011
8. M. Pisarra,  
*Studies of electron emission in the interaction of electrons with graphene on Ni(111) surface*,  
Nanoscience & Nanotechnology 2011, 19-23 Sep 2011, Frascati, Rome

9. V. Pingitore M. Barberio, P. Barone, A. Bonanno, A. Oliva,  
*Transport properties of alkali -doped single -wall carbon nanotubes mats*,  
Nanoscience & Nanotechnology 2011, 19-23 Sep 2011, Frascati, Rome

## **E.2 Presentations at national conferences in 2011**

1. P. Sapia,  
*Il ferromagnetismo: Case study basato sulla metodologia PEC*,  
50° Congresso Nazionale dell'Associazione per l'Insegnamento della Fisica - AIF'' – Piacenza – 19-  
22/10/2011.

## 4. EXPERIMENTAL PARTICLE PHYSICS

### *Professors and*

*Researchers* M. Capua  
G. Crosetti  
L. La Rotonda  
A. Mastroberardino  
M. Schioppa  
G. Susinno  
E. Tassi

*Postdoc fellows* A. Policicchio  
D. Salvatore  
T. Venturelli

*PhD students* V. Lavorini  
A. Milazzo  
V. Scarfone

*Technicians:* F. Pellegrino, V. Romano, P. Turco

Experimental particle physics studies the fundamental constituents of matter and the forces that cause their mutual interactions by means of particles accelerators and detectors. A particles accelerator is a device that uses electromagnetic fields to propel charged particles to high energy (in the most powerful accelerators the energy reaches 14 TeV). There are two ways to use these devices: sending the accelerated particles towards a fixed target, accelerating two beams of particles directed against one to each other. A particle detector is a device used to detect, track and identify high energy particles produced by the reactions in a particle accelerator. The innovative technologies used for these studies have wide implications in many fields of science (medicine, biology, informatics, etc.).

The researches on high energies physics to which the physicists of University of Calabria take part are:

1. Study of the proton structure in deep inelastic scattering processes with the ZEUS experiment at the lepton-proton accelerator HERA of the DESY Laboratory (Hamburg, Germany).
2. Study of proton-proton interactions with the ATLAS experiment at the LHC accelerator of the CERN Laboratory (Geneva, Switzerland).
3. Study of a forward physics detector for ATLAS experiment (AFP) and for medical applications.
4. R&D of hadronic calorimeter modules based on the Dual Readout Method (DREAM).
5. Study of the electron-positron interactions at the centre of mass energy 1020MeV with KLOE apparatus at DAFNE collider of LNF Laboratory (Rome, Italy).
6. Study with a ground-based apparatus of the showers produced by very high energy cosmic rays (UNICAL, Italy).

### 4.1 THE ZEUS EXPERIMENT AT THE HERA E-P COLLIDER (DESY, HAMBURG-GERMANY)

*Physicists:* M. Capua  
A. Mastroberardino  
M. Schioppa  
G. Susinno  
E. Tassi

*Technicians:*

*International collaboration*

ZEUS is a collaboration running a large particle detector at the electron-proton collider, HERA, at the DESY laboratory in Hamburg. The participating scientists are pushing forward our knowledge of the fundamental particles and forces of nature, gaining unsurpassed insight into the exciting laws of the microcosm. The ZEUS detector was a sophisticated tool for studying the particle reactions provided by the high-energetic beams of the HERA collider. At the HERA collider two separate magnet systems guided the electron ( $e$ ) and proton ( $p$ ) beams around the 6,3 km long ring and two independent superconducting RF systems accelerated the  $e$  and  $p$  bunches up to 30GeV and 920GeV energy respectively.

The High Energy Experimental Physics (HEP) group of the UNICAL has been involved in the ZEUS Collaboration, since 1988, in the design, construction, testing, calibration, alignment, running and maintenance of three components of ZEUS experiment: Forward Muon Spectrometer (FMUON), Leading Proton Spectrometer (LPS) and MicroVertex (MVD). Furthermore the UNICAL HEP researchers participate, since 1991 when the detector started operating, to the data taking as well as the physics analyses.

At the maximum beam energies the centre of mass energy is  $\sim 320\text{GeV}$ , much larger than previously achieved in such collisions, and allowing to probe the proton structure down to distance scales as low as  $10^{-18}\text{m}$  which is a factor 1000 smaller than the proton radius. With this resolving power exciting physics topics can be studied, such as proton structure, neutral and charged current processes, tests of Quantum Chromodynamics, studies of diffraction and searches for physics beyond the Standard Model. At large momentum transfers (the kinematical limit at HERA is  $10^5\text{GeV}^2/c^2$ ) there is a direct interaction of the electron with one of the quarks in the proton. For this reason HERA is often addressed as the world's only lepton-quark collider.

ZEUS collected 0.5fb-1 of data and new results are in progress and the UNICAL members of the Collaboration are actively involved in data analysis. In particular during the 2011 year we have continued to contribute to:

- the combination of the ZEUS and H1 inclusive results and determination of the proton parton distribution functions;
- the studies of Deeply Virtual Compton Scattering in diffractive processes with the complete HERA data set (see fig. 1).

One of the most important goal of the HERA research program is to capitalise the experience gained in the study of inclusive and diffractive processes and apply it to the measurements at the LHC experiments.

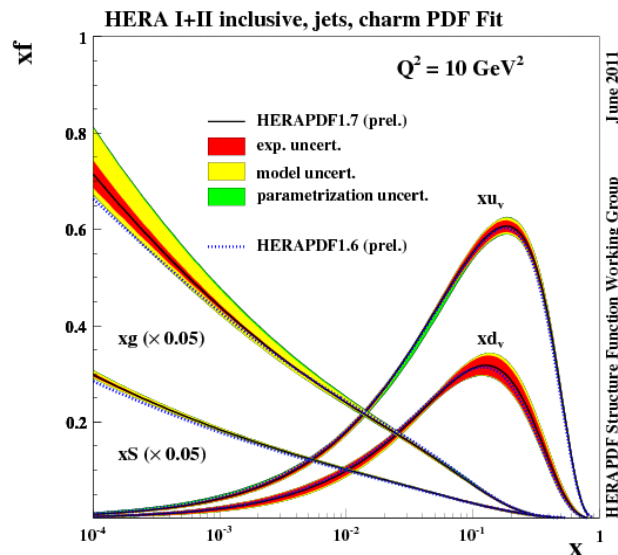


Fig. 1 Proton parton distribution functions determined from the combination of the H1 and ZEUS combined data.

#### 4.2 ATLAS Experiment at the LHC proton-proton collider (Geneva – Switzerland)

*Physicists:*

- G. Crosetti
- M. Capua
- L. La Rotonda
- V. Lavorini
- A. Mastroberardino
- A. Milazzo
- A. Policicchio
- D. Salvatore
- V. Scarfone
- M. Schioppa
- G. Susinno
- E. Tassi
- T. Venturelli

*Technicians:* F. Pellegrino, V. Romano, P. Turco

Nature has given us more than one elementary particle (6 leptons, 6 quarks and the carriers of the four fundamental interactions), whose masses range in a wide interval of values from the mass-less photon to the top quark mass,  $M_t=170 \text{ GeV}/c^2$ . The mechanism that determines the particle masses is still unknown and many experiments with particle accelerator have been undertaken to give an insight into it and explain the mass origin.

In 1964 Peter Higgs first proposed a clever solution to this puzzle: an undetectable field, similar to the electromagnetic one, permeates the whole space. As particles move in space they travel through this field, and interaction with this field allows them to acquire their masses. This is similar to the action of viscous forces felt by particles moving through any thick liquid: the stronger the interaction of the particles with the field, the bigger the mass they seem to have. We know from quantum theory that fields have particles associated with them, so a Higgs boson should be associated to the Higgs field. Up to now no one has ever observed the Higgs boson in an experiment to confirm the theory. Finding this particle would give an insight into why particles have certain mass, and help to develop subsequent physics. The technical problem is that we do not know the mass of the Higgs boson itself, which makes it more difficult to identify. Physicists have to look for it by systematically searching a range of mass within which it is predicted to exist. The yet unexplored range is accessible using the Large Hadron Collider (LHC). Fig. 2 shows a preliminary result recently presented by the Collaboration.

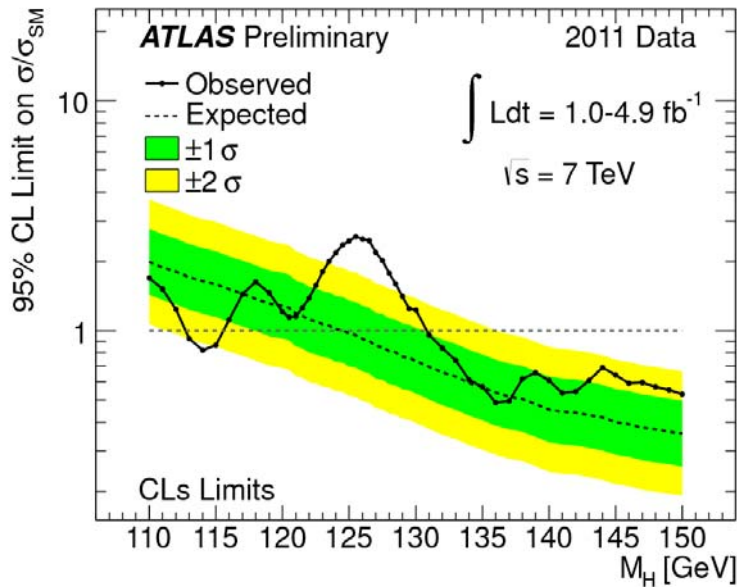


Fig. 2 Experimental limits from ATLAS on Standard Model Higgs production in the mass range 110-150 GeV. The solid curve reflects the observed experimental limits for the production of Higgs of each possible mass value (horizontal axis). The region for which the solid curve dips below the horizontal line at the value of 1 is excluded with a 95% confidence level (CL). The dashed curve shows the expected limit in the absence of the Higgs boson, based on simulations. The green and yellow bands correspond (respectively) to 68%, and 95% confidence level regions from the expected limits.

This collider provides 10 times higher center of mass energy and 100 times higher p-p collision rates than Tevatron collider and is fully operational since November 2009. This opens up a new frontier of physics and the LHC experiments, ATLAS, CMS, ALICE and LHCb, are ready to explore this great potential.

ATLAS is a general-purpose experiment. Designed to see a wide range of particles and phenomena produced in LHC collisions, it involves approximately 2500 physicists and engineers from some 35 countries. These scientists use the data collected from the complex detectors to search for new phenomena, including the Higgs boson, super-symmetry and extra dimensions. They also measure the properties of previously-discovered quarks and bosons with unprecedented precision, and are on the lookout for completely new, unpredicted phenomena. The basic design concept to achieve these goals includes three detector systems (fig. 3):

0. the *inner tracker*, with semiconductor pixel and strip detectors for very high accuracy measurements of the charged particle trajectories, followed by straw tube detectors giving independent electron identification. The tracker is confined to a cylinder 6.8 m long and with a radius of 1.1 m in a 2 T magnetic field, provided by a superconductive solenoid;

1. the *calorimeter*, with an inner cylinder in highly granular liquid argon technology with Pb absorber, followed at large radius by an iron-tile scintillator calorimeter providing good resolution in a very cost-effective manner;
2. the high precision standalone *muon spectrometer*. Its conceptual layout is based on the magnetic deflection of muon track in a system of three large superconducting air-core toroid magnets instrumented with separate-function trigger and high-precision tracking chambers.

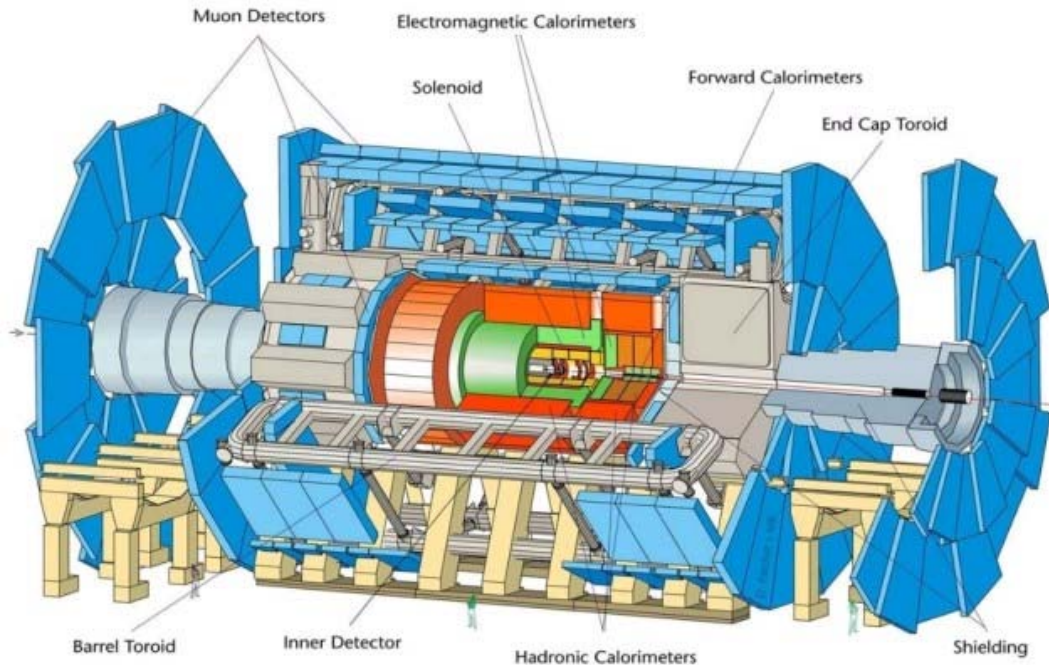


Fig. 3 Overview of the ATLAS detector.

The researchers of the experimental high energy physics (HEP) group of UNICAL have been strongly involved in various aspects of the design, construction, installation and test of the muon spectrometer since 1994. During this period the contribution from many undergraduate, graduate and PhD students and postdoc researchers has been substantial to this end.

During 2011 the Unical HEP group gave a major contribution to the following ATLAS activities:

1. Participation in the maintenance and improvement task force of the muon precision chambers at CERN. This is a group of expert physicists taking care of the whole detector performance, overlooking the functionality of gas, readout, alignment, data control, high and low-voltage systems.
2. Development and maintenance of the Gnam package, the low-level data acquisition software for the ATLAS sub-detector online monitoring. This tool has been developed since 2004 for the combined test beam of a slice of the ATLAS Muon Spectrometer. It was highly appreciated and widely used during the installation and commissioning phase of the spectrometer and has been inserted into the official Trigger and Data Acquisition software of the ATLAS experiment. At the moment most of the ATLAS sub-detectors use Gnam online histograms to evaluate the quality of acquired data. In fact it is capable to promptly spot if sub-detectors are not working properly. It decodes the raw data coming from sub-detectors and shows the relevant quantities through histograms. As an example, it reveals dead or noisy channels, which may affect the data taking itself and subsequent reconstruction and pattern recognition processes.
3. Development of a JAVA program for the online monitor of RPC detector (RPC GNAMon). This program allows to check few minutes after the start of the data run the status of the barrel RPC chambers. It produces an overview panel where all the chambers are shown. Depending on the average rate of the chamber it appears with a specified colour. Clicking on the chamber a panel with all details appear.
4. Design and simulation of the ATLAS Forward Physics (AFP) apparatus. The AFP is a proposed project which comprises a new generation of 3D silicon detectors, to be inserted along the beam pipe, at a distance of 220 m and 420 m from the interaction point. The installation of the detectors will allow the ATLAS experiment to study diffractive processes including the very important diffractive production of the Higgs boson.
5. Study of the W and Z bosons and top quark production. This study constitutes an important part of the ATLAS physics program at the LHC. The measurement of their large production cross sections, that are known at the next-to-next-to-leading order (NNLO) in QCD, will allow to perform stringent tests of the predictions of the Standard



Model and to study the properties of the gauge bosons in a hitherto unexplored kinematics region. The study is performed via the measurement of the W and Z bosons production cross-sections in the leptonic channels with the data collected by the ATLAS detector in the years 2010 and 2011. Another topic of interest is the precise measurement of the W and Z charge asymmetry that could improve our understanding of the proton's parton distribution functions, when included in Altarelli-Parisi QCD fits. The top quark, the heaviest of all known elementary particles, was discovered in 1995 at the Fermilab Tevatron collider. Studying top quarks is important for several reasons. With its large mass, the top quark is the only fermion at the electroweak scale; it is therefore of great interest for the studies of electroweak symmetry breaking. Moreover measuring accurately the top quark mass helps to put constraints on the SM Higgs boson mass. Additionally, top quarks will constitute a significant background process to many beyond SM searches. The very last study in this topic is the top pairs production in the semileptonic channels, where events in the electron/muon plus jets channel are isolated.

6. Study of the Long-Lived particles of the Hidden Valley sector. Several extensions of the SM predict the existence of neutral, weakly coupled unstable particles with macroscopic decay lengths. Among these the Hidden Valley (HV) scenario predicts neutral long-lived particles, the so-called  $\nu$ -pion ( $\pi_\nu$ ), that decay to fermion pairs. These particles can be produced in Higgs boson decays, supersymmetric processes and  $Z'$  decays. At the time of design, the ATLAS apparatus was not optimised to reveal neutral particles with long decay paths and final states displaced throughout the overall detector and, therefore, these events should be undetected. The study of the ATLAS detector performances for the Higgs boson decays in final states of the hidden sector is underway, in collaboration with the INFN/University of Rome1 and the Seattle University of Washington. The muonic decay channel represents the favourite decay mode and has a very clean topological signature. The analysis has been performed using 1.94 fb<sup>-1</sup> of collision events collected during 2011 and no excess of events is observed above the expected background. The limits on the Higgs boson production times branching ratio decaying to neutral long-lived lepton jets are derived as a function of the particle proper decay length. The  $\pi_\nu$  decays in the hadronic calorimeter and it is tagged using one of the *ad-hoc* trigger algorithms developed for this purpose. The analysis, based on the full available statistics collected by the ATLAS detector in 2011, focuses on the studies of Monte Carlo signal and main background sources (QCD, Cosmics and Beam Halo events) to choose a proper set of variables that allow us to discriminate between signal and background.

### 4.3 HADRONIC CALORIMETRY

*Physicists:* L. La Rotonda  
A. Policicchio  
G. Susinno  
T. Venturelli

*Technicians:* F. Pellegrino, V. Romano

*International collaboration*

High-precision measurements of hadrons and hadron jets have become increasingly important in experimental particle physics. The energy resolution of a hadron calorimeter is in general much worse than what can be achieved for e.m. shower detection. The wide variety of possible interaction processes and the effects associated with excitation of the absorber nuclei are considered responsible for this.

In compensating hadron calorimeters a dominant source of fluctuations that comes from  $\pi^0$  production in the shower is eliminated by equalising the calorimeter response to e.m. and purely hadronic shower component.

In recent years, R. Wigmans (Texas Tech) in collaboration with other groups have developed an alternative technique: The Dual Readout Method (DREAM). DREAM calorimeters are based on a simultaneous measurement of different types of signals which provide complementary information about details of the shower development.

The DREAM prototype, that has been successfully tested at CERN, is a copper absorber structure, equipped with two types of active media. Scintillating fibres measure the total energy deposited by the shower particles, while Quartz fibres measure the Cerenkov light that is only produced by the charged, relativistic shower particles.

Since the latter are almost exclusively found in the e.m. shower component (dominated by  $\pi^0$  s produced in hadronic showers), a comparison of the two signals makes it possible to measure the energy fraction carried by this component, fem, event by event.

Once the effects of the dominant source of fluctuations, *i.e.*, fluctuations in the e.m. energy fraction fem, are eliminated, the performance characteristics are determined (and limited) by other types of fluctuations. In the described detector, a prominent role is played by the small number of Cerenkov photoelectrons constituting the signals (8 p.e./GeV) due to the small sampling fraction used in the prototype.

Moreover, for the measurement of electromagnetic showers and photons, it could be convenient to place in front to a DREAM-like calorimeter a high resolution electromagnetic homogenous calorimeter. In such a calorimeter it would be

important to preserve the possibility of dual readout in order to correct the energy measurement of the fraction of hadrons developing electromagnetic showers already in this detector.

So, in order to improve the DREAM setup different ways are practicable:

- a) Increase the sampling fraction in DREAM-like calorimeters, to increase the light collected
- b) production of crystal electromagnetic calorimeters with dual readout to be placed in front of DREAM-like calorimeters, to improve the energy resolution of electromagnetic showers, keeping the possibility of measuring the electromagnetic fraction of hadrons showers that start in the electromagnetic calorimeter that can then be compensated on an event-by-event basis.

To this last projects, with U.S. researchers an Italian collaboration: Bologna - Cagliari - Cosenza - Roma1 -Pavia is working from 2006.

In a homogeneous calorimeter the two light components can be disentangled by:

- (1) Directionality. The Cerenkov light is emitted at a fixed angle with respect to the momentum vector of the particle that generates it, while the scintillation light is isotropically emitted.
- (2) Time structure. The Cerenkov light is prompt, whereas scintillation processes have one or several characteristic decay times.
- (3) The spectrum. The Cerenkov light is emitted with a characteristic  $\lambda^{-2}$  spectrum, while the scintillation processes have their own characteristic spectra.
- (4) Polarization. Contrary to scintillation light, Cerenkov light is polarized.

Very promising results have been obtained in case of single doped BGO crystals and a small electromagnetic calorimeter made of lead tungstate (PbWO<sub>4</sub>) crystals tested in conjunction with the DREAM calorimeter mentioned above, and exposed to high energy particle beams at CERN's Super Proton Synchrotron.

Time structure and spectrum of signals like to be the most interesting characterisation of two signals.

The study of new crystals more efficient to discriminate scintillation and Cerenkov light and the development of a faster electronic are going on.

The last additional feature that might in principle be used to distinguish scintillation from Cerenkov light is the fact that the latter is polarized. In 2010 we investigated the possibilities in this respect. High-energy pions were used to generate signals in a BGO crystal, and the effects of polarization filters on the two types of light generated in this crystal have been measured.

Respect to point a) in 2010 the first four prototype modules of a new DREAM-like calorimeter have been constructed and successfully tested. Prototype construction is going on and in 2011 they have been tested.

MIUR has considered this project as a PRIN (Progetto di Ricerca di Interesse Nazionale) project and has funded it in the period 2010-2012

In summer 2011 this R&D (Research and development experiment) has been accepted as an official CERN R&D experiment.

The Cosenza researchers participate to the Test Beam, data analysis and to the new modules construction and are successfully involved in the Geant simulation of the detector.

#### 4.4 3D PIXEL COLLABORATION

*Physicists:*  
M. Capua  
A. Mastroberardino  
G. Susinno

*International collaboration*

The 3D pixel Collaboration was approved in July 2007 and includes 4 processing facilities: CNM Barcelona (Spain), FBK Trento (Italy) and the 3DC Consortium with SINTEF (Norway) and Stanford (USA). The main goals of these studies are the development, industrial fabrication, characterisation and testing, with and without front-end readout chips, of full-3D with active-edge and mod (double side)-3D silicon pixel sensors of extreme radiation hardness and high speed for the Super-LHC ATLAS upgrade and the ATLAS B-layer replacement (IBL).

A specific goal is to demonstrate the design implementations of 3D as a safe sensor solution for the IBL in the high radiation environment expected during the full period between the LHC phase-1 and phase-2 upgrades.

#### 4.5 KLOE-2 EXPERIMENT AT DAFNE E-E+ COLLIDER (National Laboratory of Frascati)

*Physicists:* M. Schioppa

*International collaboration*

The DAFNE collider accelerates stores electrons and positrons of 510MeV energy each to produce PHI-mesons via the reaction  $e^+e^- \rightarrow \gamma^* \rightarrow \text{PHI}$ . This meson is made of strange – anti-strange quarks; has 1020 MeV/c<sup>2</sup> mass and has the quantum numbers of the photon:  $J^{PC} = 1^{--}$ . It decays at rest and the final state contains mainly charged and neutral kaon pairs (branching ratio BR=49.5% and BR=34.3% respectively), RHO-PI and PI+PI-PI0 (BR=15.5%), ETA-GAMMA (BR=1.3%), ETA'-GAMMA (BR=0.00012). The neutral kaon pairs are produced in a well-defined quantum and kinematical state with negative charge parity. The kaons are monochromatic (the momentum is 127MeV/c for charged kaons and 110MeV/c for the neutral one) and are emitted back to back to be detected in an almost background free environment. With the integrated luminosity of 2.5fb<sup>-1</sup> (2001-2006) the collider has produced 10<sup>10</sup> PHI-mesons and than about 10<sup>10</sup> kaon pairs.

The experiment KLOE is a general purpose detector designed to study all kinds of kaon, PHI, RHO, ETA and ETA' decays emphasising tests of discrete symmetries (CP-, CPT-, T-invariance) and measurements of hadronic cross sections and tests of chiral perturbation theory.

The detector is a huge (4m diameter, 4m long), transparent drift chamber in 0.5Tesla magnetic field produced by a super-conductive solenoid, with 55000 stereo wires, in helium based gas mixture, surrounded by a lead-scintillating fibre calorimeter, 15X0 thick, 98% solid angle coverage with a resolution of 54ps/SQRT(E)+140ps (E in GeV) in time and 5.7%/SQRT(E) in energy.

During 2008 the INFN has approved the KLOE-2 proposal at the improved DAFNE luminosity performance. The data taking campaign (20-50fb<sup>-1</sup>) started on spring 2011.

The contribution to KLOE-2 project of the UNICAL's researcher has been focused on CCALT LYSO calorimeter performance studies using GEANT4 simulations, QCALT tile calorimeter tests with UV pulsed LED on photodiodes, tiles and fibres, cylindrical GEM inner tracker detector construction and test and the study of light boson weekly coupled with standard matter using initial state radiation events.

#### 4.6 AIR SHOWER OBSERVATORY WITH SCINTILLATOR DETECTORS ARRAY

*Physicists:* M. Schioppa

During the last 20 years the Astroparticle research has considerably contributed to the better understanding of the laws that govern the Universe but it has also left many open questions (i.e. the origin, the acceleration mechanism and the elementary composition of the Cosmic Rays) that can be coped only with ground based experimental apparatus that are the only capable to detect those CR coming from galactic and extra-galactic exotic astrophysical sources and directly from the Big Bang. Indeed these particles have energy greater than 100TeV (UHE) and interact with the nuclei of the atmosphere generating extensive air showers (EASs). During the last years the ground-based apparatus have reached goals unattainable with the other techniques to explore the Universe. For example it has put in evidence a very large number of gamma-sources from our galaxy and from other galaxy, it has demonstrated the existence of very complex gamma sources, and it has discovered extra-galactic gamma source at distance never explored previously.

The researchers of UNICAL physics department, with the precious collaboration of physics students, have designed and realised an EAS observatory made of 3 large scintillator counters placed at the vertex of an equilateral triangle, 20m side. The apparatus detects EAS produced by CR of energy greater than PeV and can measure the direction of the primary CR with a resolution of 5°. The apparatus is particularly suitable also for didactics purpose.

## A PUBLICATIONS ON SCIENTIFIC JOURNALS

### A.1 Publications on international scientific journals

#### A.1.1 Publications on international scientific journals published on 2011

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2. La Rotonda L., Policicchio A., Susinno G., Venturelli T., DREAM C.,  
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*Measurement of Dijet Azimuthal Decorrelations in pp Collisions at  $\sqrt{s}=7$  TeV.*  
Phys.Rev.Lett. 106 (2011) 172002
46. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Search for supersymmetry using final states with one lepton, jets, and missing transverse momentum with the ATLAS detector in  $\sqrt{s} = 7$  TeV pp.*  
Phys.Rev.Lett. 106 (2011) 131802
47. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Search for Massive Long-lived Highly Ionising Particles with the ATLAS Detector at the LHC.*  
Phys.Lett. B698 (2011) 353-370
48. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Luminosity Determination in pp Collisions at  $\sqrt{s}=7$  TeV Using the ATLAS Detector at the LHC.*  
Eur.Phys.J. C71 (2011) 1630
49. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Study of Jet Shapes in Inclusive Jet Production in pp Collisions at  $\sqrt{s} = 7$  TeV using the ATLAS Detector.*  
Phys.Rev. D83 (2011) 052003
50. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Measurement of the production cross section for W-bosons in association with jets in pp collisions at  $\sqrt{s} = 7$  TeV with the ATLAS detector.*  
Phys.Lett. B698 (2011) 325-345
51. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Measurement of the centrality dependence of  $J/\psi$  yields and observation of Z production in lead-lead collisions with the ATLAS detector at the LHC.*  
Phys.Lett. B697 (2011) 294-312
52. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Measurement of the inclusive isolated prompt photon cross section in pp collisions at  $\sqrt{s} = 7$  TeV with the ATLAS detector.*  
Phys.Rev. D83 (2011) 052005
53. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Charged-particle multiplicities in pp interactions measured with the ATLAS detector at the LHC.*  
New J.Phys. 13 (2011) 053033
54. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Search for Diphoton Events with Large Missing Transverse Energy in 7 TeV Proton Proton Collisions with the ATLAS Detector.*  
Phys.Rev.Lett. 106 (2011) 121803
55. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.



*Measurement of the top quark-pair production cross section with ATLAS in pp collisions at  $s\sqrt{=7\text{ TeV}}$ .*  
Eur.Phys.J. C71 (2011) 1577

56. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Measurement of underlying event characteristics using charged particles in pp collisions at  $s\sqrt{=900\text{GeV}}$  and 7 TeV with the ATLAS detector.*  
Phys.Rev. D83 (2011) 112001
57. Capua M., Crosetti G., La Rotonda L., Mastroberardino A. Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Search for Quark Contact Interactions in Dijet Angular Distributions in pp Collisions at  $\text{sqrt}(s) = 7\text{ TeV}$  Measured with the ATLAS Detector.*  
Phys.Lett. B694 (2011) 327-345
58. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.  
*Measurement of inclusive jet and dijet cross sections in proton-proton collisions at 7 TeV centre-of-mass energy with the ATLAS detector.*  
Eur.Phys.J. C71 (2011) 1512
59. M. Capua, A. Mastroberardino, G. Susinno, ATLAS 3D C.  
*3D-FBK pixel sensors: Recent beam tests results with irradiated devices.*  
Nucl.Instrum.Meth. A650 (2011) 150-157
60. M. Capua, A. Mastroberardino, G. Susinno, ATLAS 3D C.  
*Test Beam Results of 3D Silicon Pixel Sensors for the ATLAS upgrade.*  
Nucl.Instrum.Meth. A638 (2011) 33-40
61. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., ZEUS C.  
*Study of tau-pair production at HERA*  
JHEP 1102 (2011) 117.
62. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., ZEUS C.  
*Measurement of beauty production in deep inelastic scattering at HERA using decays into electrons*  
Eur.Phys.J. C71 (2011) 1573.
63. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., ZEUS C.  
*Measurement of heavy-quark jet photoproduction at HERA*  
Eur.Phys.J. C71 (2011) 1659.
64. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., ZEUS C.  
*Measurement of the t dependence in exclusive photoproduction of Upsilon(1S) mesons at HERA*  
Phys.Lett. B708 (2012) 14-20.
65. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., ZEUS C.  
*Scaled momentum distributions for  $K^0_S$  and  $\Lambda^0$  in DIS at HERA*  
JHEP 1203 (2012) 020.
66. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., ZEUS C.  
*Search for single-top production in  $ep$  collisions at HERA*  
Phys.Lett. B708 (2012) 27-36.
67. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., ZEUS C.  
*Exclusive electroproduction of two pions at HERA*  
Eur.Phys.J. C72 (2012) 1869.

### **A.1.2 Publications on international journals accepted in 2011**

### **A.1.3 Public international notes in 2011**

1. A. Policicchio, M. Schioppa, et al., *A search for Long Lived Lepton-Jets from Higgs decay in the ATLAS detector*, ATL-COM-PHYS-2011-1365 Geneva CERN, 2011.
2. A. Policicchio et al., *Search for Light Higgs Decay to Long-lived Neutral Particles*, ATL-COM-PHYS-2011-956.- Geneva : CERN, 2011.
3. A. Policicchio et al., *Triggers for Long Lived Neutral Particles in the ATLAS apparatus*, ATL-COM-PHYS-2011-945.- Geneva : CERN, 2011.
4. A. Policicchio et al., *Performance of the ATLAS Muon Trigger in p-p collisions at  $\sqrt{s} = 7$  TeV*, ATLAS-COM-CONF-2011-099.- Geneva : CERN, 2011

## **B PUBLICATIONS ON CONFERENCE PROCEEDINGS**

### **B.1 Publications on international conference proceedings in 2011**

1. M. Capua, for the H1 and ZEUS Collaborations, *DVCS and VM at HERA*. MPI11 3rd International Workshop on Multiple Partonic Interactions at the LHC 21.11.2011 - 25.11.2011 DESY, Hamburg. Proceedings arXiv:1202.2828 [hep-ex], [www-ekp.physik.uni-karlsruhe.de/pub/pic2010/proceedings/025\\_Marcella\\_Capua.pdf](http://www-ekp.physik.uni-karlsruhe.de/pub/pic2010/proceedings/025_Marcella_Capua.pdf), 7pp.
2. A. Policicchio et al., *Boosted objects as a probe of beyond the standard model physics*, Prepared for BOOST 2010 Oxford, England (2010), Eur. Phys. Jour. C71, 1 (2011).
3. A. Policicchio et al., *Search for Long-Lived particles in ATLAS detector*, Prepared for IFAE 2011, Perugia, Italy (2011), NCC34, 272 (2011).

## **PRESENTATIONS AT SCHOOLS AND CONFERENCES**

### **C.1 Invited presentations at international schools and conferences in 2011**

1. Marcella Capua (ZEUS): *DVCS and VM at HERA*  
MPI11 3rd International Workshop on Multiple Partonic Interactions at the LHC 21.11.2011 - 25.11.2011 DESY, Hamburg.
2. Enrico Tassi (ZEUS): *Structure function measurements at HERA and their impact for LHC*, LLWI2011 Lake Louise Winter Institute 20.02.2011 - 26.02.2011 Lake Louise, Canada.
3. Policicchio and D. Salvatore: *Search for Long-Lived Neutral Particles in ATLAS Detector*, poster presented at 49th International School of Subnuclear Physics, Erice, June 24th - July 3rd 2011.
4. A. Policicchio, *LLNP decays in ATLAS Calorimeter*, ATLAS LLP workshop, Roma, Italy (2011).
5. A. Policicchio, *Search for Long-Lived particles in ATLAS detector*, IFAE 2011, Perugia, Italy (2011).

## 5. GEOPHYSICS

<i>Professors and Researchers:</i>	I. Guerra A. Gervasi ( <i>Researcher from National Institute of Geophysics and Volcanology (INGV)</i> )
<i>PhD Student:</i>	M. Anzidei
<i>Postdoc fellows:</i>	B. Orecchio
<i>Technical staff:</i>	L. Festa, G. Latorre
<i>Collaborators:</i>	A. Moretti ( <i>Univ. of L'Aquila, L'Aquila, Italy</i> ) G. Neri, D. Presti, and C. Totaro ( <i>Univ. of Messina, Messina, Italy</i> ) W.J. Kim, A. Lerner-Lam, L. Seeber, C. Stark and M. Steckler ( <i>Lamont-Doherty Observatory, Columbia Univ., New York, USA</i> ) M. Nedimovic ( <i>Halifax Univ., Canada</i> ) V. Carbone, A. Vecchio, P. Veltri, G. Zimbaro ( <i>Calabria Univ., Arcavacata, Italy</i> ) L. Sorriso-Valvo ( <i>LICRYL, INFN/CNR, Cosenza</i> ) S. D'Amico ( <i>Physics Department, University of Malta</i> ) A. Benini ( <i>archaeologist</i> ) G. Corrado and A. Albano ( <i>Federico II University, Naples, Italy</i> ) C. Faccenna, A. Billi, L. Minelli ( <i>RomaTre University</i> )
<i>Institutional scientific agreements:</i>	National Institute of Geophysics and Volcanology (Rome) Lamont-Doherty Earth Observatory (Palisades, New York, USA)

## RESEARCH LINES

### Introduction

In spite of its lean composition, the Geophysics Research Group is engaged in many lines of activity. In most cases this is due to the nature of its activities, based on the elaboration of experimental data collected by means of observations that have to be carried on over long span of time. The research group in Geophysics at the Calabria University was indeed established more than thirty years ago in a department different from Physics with the explicit finality of answering the requirement of seismological observations in Calabria, a region characterized by a seismic risk level among the highest in the Mediterranean Basin. This origin is still conditioning its programs, mainly of observational nature.

Due also to the relatively great distance from the nearest centres of geophysical research and the relevance of the geodynamical problems arising from the features of the territory, the group at the Department of Physics is a reference point for both researchers, from abroad too, as well as some public administrations.

### 5.1 Seismotectonics

Seismotectonics is the branch of seismology that deals with the complex relations between earthquakes and geological structures and with the reconstruction of the ongoing dynamical processes. It is based on the accurate location of the seismic sources, that in turn requires a model as more realistic as possible for the elastic waves propagation in the studied area. Generally, an iterative process is performed: new seismographic data help to better constrain the velocity model that in turn leads to better locations. The maps of seismicity resulting from the above mentioned activity is then correlated to the tectonic features observed in the area. In particular the space distribution of the seismic foci can trace the position of the slip surfaces at depths not accessible to direct observation, while the propagation model includes the mechanical discontinuities met with by seismic waves along their path to the seismic stations. Seismograms contain further information that allows for determining the dynamics of the phenomena at the seismic sources. The reconstruction of the geometry of the geological bodies and their present kinematics is the result of these research activities.

Accurate seismotectonic investigations are essential in Calabria because of the peculiarity of seismic activity in the region. The area hosted in fact most of the largest earthquakes reported in Italy in historical times. However it has been practically quiescent since 1908. Moreover the adjacent Tyrrhenian Sea is the seat of deep earthquakes attributable to the complex interaction of the Eurasian and African lithospheric plates, that includes the so-called subduction phenomenon namely the sinking of the southern continent beneath the northern one. The present day stage of this

process in comparison to the analogous ones observed worldwide and further specific details make Calabria one of the most interesting geodynamical problems in the Mediterranean area. Therefore the geophysical monitoring of the local seismicity and associated phenomena and their relation to the tectonic features are an important task for the scientific investigation devoted to both the pure geophysics and the seismic risk assessment.

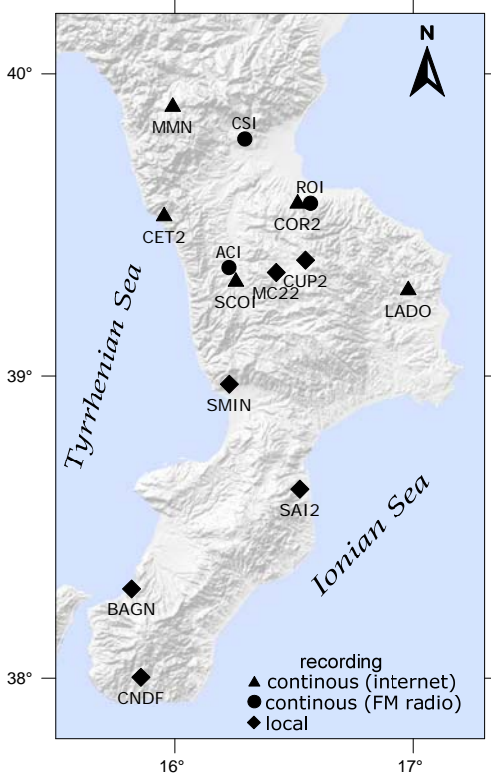


Fig 1 - The Calabria University seismic network (2011).

The seismic sequence started in Autumn of 2010 on the northern slope of the Pollino Range (Northern Calabria and Southern Basilicata regions) continued in 2011, showing frequent migrations of the area of maximum seismic energy release. This could indicate the activation in succession of different segment of possibly more than one fault. In particular at the end of October a new tectonic structure was interested, and new populations were involved, this time in the adjacent Basilicata Region. As a consequence, the seismic monitoring apparatus was further upgraded. Five temporary seismographs were made available by INGV and installed in addition to the previous ones, both on the northern slope of the Pollino chain and in Calabria

At the time of this report, the sequence is still continuing and the main source of seismic energy moved sharply on the southern slope of the Pollino chain, where on May 28, 2012, an earthquake occurred with local magnitude  $m_L = 4.3$ , the maximum since its beginning.

A huge quantity of data has been acquired till now and is still increasing, so that their collection and organization hinder the successive phases of the work. However, historical evidence has been found that similar sequences occurred in the past at intervals of several decades. This makes a must the long ongoing observation campaign, according to the principle that in seismology all data not-recorded are lost data.

In this frame, most of the daily effort of the research group is devoted to the management of the Calabria Regional Seismic Network (Fig. 1). This network has the dual role of providing an almost real time monitoring of the area and of incrementing the available waveform data bank. The first is useful in civil protection tasks, the collected information being sent to National Institute of Geophysics and Volcanology, Rome (INGV); the second is the basic instrument to carry on seismotectonic investigations.

In 2011 continued therefore the efforts in the reorganizing and enhancing the permanent Calabria Seismic Network. A newly established seismographic station (CET2) was added to the monitoring system, in substitution of the former SIMO. Its characteristics include broad-band sensor, 3D digital acquisition system and telematic connection for real-time recording and utilization of data. In consideration of its high quality from the seismographic point of view, its signals are sent also to the recording centre of INGV in Rome, as a new observation point of the National Seismic Network.

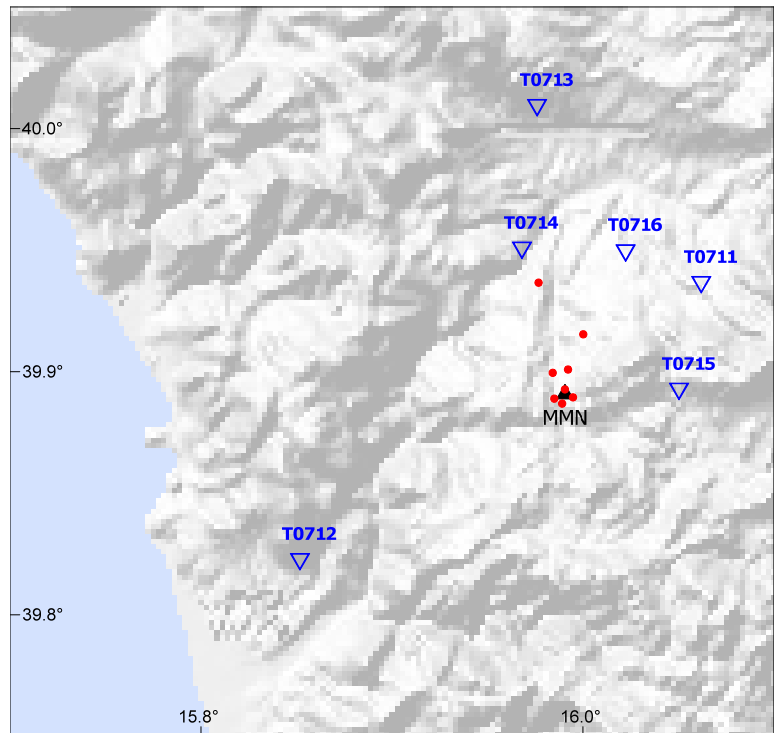


Fig. 2 – The Pollino seismic array (2011). Black triangle: the permanent station MMN; red dots: sites of UniCal seismographs; blue triangles: stations added in Autumn 2011.

## 5.2 Geodesy

Ground deformations is the geophysical phenomenon more frequently associated to the seismic activity in its various stages. It is detected by successive or continuous measurements of the coordinates of reference points (benchmarks). Both classical, optical and modern, GPS techniques can be applied.

In 2011 the Geophysical Group continued in caring the operation of the nine GPS sites installed in 2006 along the transect Cetraro-Crotone in the framework of the cooperation with the Lamont-Doherty Earth Observatory of the Columbia University (LDEO). These data gave a sound experimental basis to the paper by D'Agostino et al. (2011) born from the collaboration with INGV and LDEO.

The cooperation continued with the geologic team of the RomaTre University in Rome in order to properly frame the GPS evidences in the local geologic/seismotectonic scenario. In particular evidence has been found that allows to hypothesize a physical explanation for the eastward migration of the so-called Crotone basin relative to the Calabria itself.

The contribution by M. Anzidei to the Geophysic group in 2011 appears to be very important and fruitful. His activity allowed investigations concerning both the subsidence along the Mediterranean coasts in historical times and the behaviour of this quasi-closed basin soon after strong earthquakes. Archaeological and instrumental observations are utilized respectively in the different cases.

## 5.3 Micro-gravimetry

Gravimetry is the branch of Geophysics aimed to describe and utilize the Earth's gravity field both for scientific and commercial purposes. The values of the gravity acceleration ( $g$ ) measured near its surface differ from those corresponding to any simple model that represents the Earth as a homogeneous rotating body, due to the real inhomogeneous density distribution of materials inside our planet. The differences between the measured values of  $g$  and the theoretical ones (the so-called *gravity anomalies*) are currently used to infer information about the geometry and nature of buried rocky bodies.

Relative motions of the Earth with respect to Moon and Sun are the origin of continuous perturbations of  $g$  in any point at the Earth surface. Modern micro-gravimeters are able to record temporal variations of the order of  $10^{-8}$   $g$ . The well-known sea-tides are their most evident consequence, but the solid part of the Earth undergoes deformations like the surface of the oceans, obviously of much smaller entity.

It is possible to study these perturbations by recording the  $g$ -values and the correspondingly variable inclination of the ground. It is generally believed that, due to the periodic character of the tidal phenomena, a set of observations spanned several years should be sufficient to build a mathematical model of the behaviour of a given site. These models may be useful for studying the elastic properties of the lithosphere at a regional scale and their relationship to the structural and geodynamical context.

Microgravimetric data can be used for calculating the corrections to be applied to the observed  $g$ -values when they are measured during very detailed surveys, like those performed searching for underground voids, for example with archaeological purposes; for checking possible correlations among gravity variations and geodynamic phenomena; etc. Micro-gravimeters are also able to record the free oscillations of the Earth excited by the biggest earthquakes: these phenomena provides therefore for information about the elastic behaviour of the whole planetary body.

The *La Coste & Romberg mod. G* gravimeter and the *Applied Geomechanics mod. 712* biaxial tiltmeter provided by the Naples University were installed and started to operate in April, 2011 at the lowest floor of the building of the Calabria University where the seismological laboratory has its seat. Some technical problems have been quickly solved and the apparatus came early to its operating conditions. It will stay there for at least one whole annual cycle and after it will be moved to the Cosenza castle, its final site.

## 5.4 Dissemination and diffusion of scientific culture

Noteworthy efforts are dedicated to the diffusion of the geophysical culture, in the attempt of convincing the general public and future university students which too much frequently attribute the seismology to scientific field different from physics.

The Geophysics Laboratory is open to school visits and a set of demonstration tools is available to make geophysics understandable and appealing. Every year it is visited by hundreds of pre-university scholars.

In the framework of cooperations with Scholastic Institutes we have provided for technical assistance the Liceo Scientifico "G. B. Scorza", where a seismographic station is operating since several years. This school received in 2010 and 2011 our support in installing a meteorological station and in developing the software interface necessary to publish the measurements in real time on a properly created web-page. In January, 2011 meteorological information are also displayed in the web-site of municipality of Cosenza.

## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals in 2011**

1. Anzidei M., Antonioli F., Lambeck K., Benini A., Soussi M.,  
*New insights on the relative sea level change during Holocene along the coasts of Tunisia and western Libya from archaeological and geomorphological markers.*  
Quat. Intern., 232, 5-12, doi:10.1016/j.quaint.2010.03.018
2. Anzidei M., Antonioli F., Benini A., Lambeck K., Sivan D., Serpelloni E., Stocchi P.,  
*Sea level change and vertical land movements since the last two millennia along the coasts of southwestern Turkey and Israel.*  
Quat. Intern., 232, 13-20, doi:10.1016/j.quaint.2010.05.005
3. D'Amico S., Orecchio B., Presti D., Gervasi A., Guerra I., Neri G., Zhu L., Herrmann R.B.,  
*Testing the stability of moment tensor solutions for small earthquakes in the Calabro-Peloritan Arc region (southern Italy)*  
Boll. Geofis. Teor. Appl., 52, 2, 283-298, 2011.
4. D'Agostino N., D'Anastasio E., Gervasi A., Guerra I., Nedimović M. R., Seeber L., Steckler M.,  
*Forearc extension and slow rollback of the Calabrian Arc from GPS measurements*  
Geophys. Res. Lett., 38, L17304, doi:10.1029/2011GL048270. 2011.
5. Faccenna C., Molin P., Orecchio B., Olivetti V., Bellier O., Funicello F., Minelli L., Piromallo C., Billi A.,  
*Topography of the Calabria subduction zone (southern Italy): clues for the origin of Mt. Etna*  
Tectonics, 30, TC1003, doi:10.1029/2010TC002694, 2011.
6. Lambeck K., Antonioli F., Anzidei M., Ferranti L., Leoni L., Scicchitano G., Silenzi S.,  
*Sea level change along the Italian coast during the Holocene and projections for the future*  
Quat. Intern., 232, 250-257, doi:10.1016/j.quaint.2010.04.026
7. Orecchio B., Presti D., Totaro C., Guerra I., Neri G.,  
*Imaging the velocity structure of the Calabrian Arc region (South Italy) through the integration of different seismologic data*  
Boll. Geofis. Teor. Appl., 52, 4, 625-638, 2011.

## **D PRESENTATIONS AT CONFERENCES**

### **D.1 Presentations at international conferences in 2011**

1. D'Agostino N., D'Anastasio E., Abruzzese L., Anzidei M., Avallone A., Cardinale V., Castagnozzi, Cavaliere A., Cecere G., Cheloni D., Criscuoli F., D'Ambrosio C., De Luca G., Del Mese S., Devoti R., Esposito A., Falco L., Galvani A., Latrippa A., Massuci A., Memmolo A., Migliari F., Minichiello F., Moschillo F., Pietrantonio G., Pisani A., Riguzzi F., Selvaggi G., Sepe V., Serpelloni E., Zarrilli L., Rossi M., Mattia M., Palano M.,  
*The RING GPS network: a research geodetic infrastructure to study plate boundary deformation in the Central Mediterranean.*  
AGU Fall Meeting, S. Francisco (Poster).
2. Anzidei, M., Vecchio A., Carbone V., Arena G.,  
*Has the Mediterranean Sea Felt the March 11th, 2011, M 9.0 Tohoku-Oki Earthquake (Japan)?*  
AGU Fall Meeting, S. Francisco, abstract #U53D-0105 (Poster).
3. Anzidei M., Antonioli F.,  
*Sea Level Changes and Vertical Movements of the Land in the Mediterranean: A Review.*  
37th Interdisciplinary Workshop *The Earth Expansion Evidence: A challenge for Geology, Geophysics and Astronomy.* Intern. School Geophysics, 4 -9 October 2011, Erice.

### **D.2 Presentations at national conferences in 2011**

1. Albano A., Corrado G., Gervasi A., Guerra I.,  
*La stazione gravimetrica registratrice dell'Università della Calabria,*

30<sup>th</sup> Conv. Ann. GNGTS, Trieste, 2011.

2. Anzidei M., Antonioli F., Lambeck K., Sivan D., Soussi M., Serpelloni E., Pondrelli S., Vannucci G., Baldi P., Auriemma R., Benini A., Solinas E.,  
*Sea level changes and vertical movements of the land in the mediterranean region from integrated data*,  
Congresso AIQUA *Il Quaternario Italiano: conoscenze e prospettive* - Roma, 24-25 febbraio 2011. *Il Quaternario*,  
24, 14-16. (Abstract AIQUA, Roma 02/2011),
3. Anzidei M.,  
*Movimenti crostali e variazioni del livello del mare da dati geodetici e geofisici*,  
AIQUA Summer School: *Morfologia, geodinamica e rischio in aree costiere*. Cagliari, 12-15 settembre 2011.
4. Anzidei M., Antonioli F., Auriemma R., Benini A., Solinas E.,  
*Relative sea level changes along the Mediterranean coasts from archaeological markers*,  
Geoitalia 2011. Sessione R2. Torino, 22 settembre 2011.
5. Anzidei M., Antonioli F., Lambeck K., Sivan D., Soussi D., Serpelloni E., Pondrelli S., Vannucci G., Baldi P.,  
Auriemma R., Benini B., Solinas E.,  
*Sea level changes and vertical movements of the land in the Mediterranean*,  
Geoitalia 2011, Sessione R2. Torino, 22 settembre 2011.
6. Biolchi S., Gambin T., Abela R., Antonioli F., Furlani S., Anzidei M., Devoto S.,  
*New data on late holocene relative sea level change in Southern Malta*,  
Geoitalia 2011, Sessione R2. Torino, 22 settembre 2011.
7. Presti D., Totaro C., Gervasi A., Guerra I., Orecchio B., D'Amico S., Neri G.,  
*Focal Mechanisms in the Calabro-Peloritan Arc region*,  
30<sup>th</sup> Conv. Ann. GNGTS, Trieste, 2011.

## 6. MOLECULAR BIOPHYSICS

<i>Professors and Researchers:</i>	Luigi Sportelli Rosa Bartucci Rita Guzzi Bruno Rizzuti ( <i>Lab. LiCryL, IPCF-CNR, UOS Cosenza</i> )
<i>Post-Doc:</i>	Manuela Pantusa
<i>Student:</i>	Stefania Evoli
<i>Technical staff:</i>	Massimo Sposato
<i>Collaborators:</i>	D. Marsh ( <i>MPI for Biophysical Chemistry, Goettingen, Germany</i> ) M. Esmann ( <i>Aarhus University, Dept. of Biochemistry, Denmark</i> ) M.P. De Santo, ( <i>Dept. of Physics, Univ. Calabria and Lab. Licryl, IPCF-CNR, UOS Cosenza</i> ) B. Zappone ( <i>Lab. Licryl, IPCF-CNR, UOS Cosenza</i> ) A. Stirpe ( <i>Post-Doc</i> )

### Introduction

In the year 2011 the research activity of the Molecular Biophysics Group has essentially been focused on the study of the molecular properties of transport proteins complexed with ligands. The topic is of biophysics relevance as is strictly related to the structure/function relationship existing in biosystems. In particular, the following three research lines have been of interest of the group:

- a) Transport protein/ligand interaction
- b) Aggregation of model proteins
- c) Molecular dynamics simulation of proteins

The first research line has been approached by combining different experimental techniques such as conventional and pulsed FT-EPR, fluorescence and optical density. They allow to model the mutual influence between carrier proteins and ligands of biomedical interest.

In the second one, the catalytic effect of copper ions on the  $\beta$ -lactoglobulin fibrillation was investigated by using different experimental approaches including DSC, magnetic and optical spectroscopies and AFM.

Finally, molecular dynamics simulation has been used to investigate the binding mechanism of fatty acids to proteins such as human serum albumin and  $\beta$ -lactoglobulin and to study the role of the copper binding loop of azurin in the dynamical and thermodynamical features of the protein.

In the following, the main research results obtained during the investigation are briefly presented in the form of abstracts.

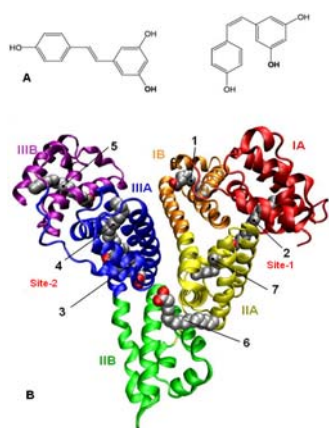
### 6.1 TRANSPORT PROTEINS/LIGANDS INTERACTION

#### 6.1.1 Interaction of the polyphenol resveratrol with human serum albumin.

Resveratrol (Fig. 1A) is a natural phytoalexin produced by some plants and it is also found in food and beverages, particularly red wine. The biological activity of resveratrol is associated with health benefits including anti-tumour, anti-inflammatory, anti-oxidant properties that make it particularly interesting for applications in pharmaceutical and nutraceutical fields. The activity and bioavailability of resveratrol, however, are limited by its low solubility in water. These limitations are overcome via binding to proteins.

Human serum albumin (HSA) (Fig 1B) is the principal extracellular protein and is reported to bind resveratrol in the site-1 specific for drugs. It also binds, stores and transports a wide variety of exogenous and endogenous molecules. In particular, it shows a strong affinity to bind reversibly and non-covalently fatty acids in the binding sites (1-7). The presence of fatty acids complexed with HSA influences the binding with drug and other ligands, and cooperative and competitive interactions can be observed.





**Fig. 1:** (A) Molecular structures of (left) *trans*- and (right) *cis*-resveratrol. (B) Crystal structure of HSA

The interaction between resveratrol and HSA in the absence and in the presence of up to 6 molecules of stearic acid (SA) pre-complexed with the protein has been studied by using the intrinsic fluorescence of both HSA and resveratrol. The aim is to investigate the influence of SA on the binding affinity of the polyphenol to the protein, on the stoichiometry of resveratrol-HSA complex and on resveratrol stability in the protein upon UV irradiation. The results highlight the ability of HSA to bind and transport hydrophobic and amphiphilic ligands and to protect from degradation an important antioxidant molecule under biologically relevant conditions.

### 6.1.2 Interaction of stearic acids with $\beta$ -lactoglobulin

Beta-lactoglobulin ( $\beta$ -LG) is a member of the lipocalin protein family involved in the transport of small hydrophobic nonpolar molecules and fatty acids. The main binding site is at a central cavity, referred to as “calyx”, formed by the protein  $\beta$ -barrel sandwich. Conventional and pulsed EPR techniques of spin-labelled stearic acids (SASL) were combined with Molecular Dynamics (MD) simulation, to investigate the interaction of fatty acids with bovine  $\beta$ -LG. Stearic acid bears the nitroxide label at different position,  $n$ , along the methylene chain ( $n = 5, 7, 10, 12, 16$ ). The EPR data show that the protein affinity for spin-labeled stearic acid decreases on going from the first segments towards the terminal methyl end of the fatty acid chain. D<sub>2</sub>O-Electron Spin Echo Envelope Modulation (ESEEM) Fourier-transform spectra indicate that the spin-probe is accessible to the solvent at any position along the stearic acid chain, although the <sup>2</sup>H intensity decreases on moving toward the terminal methyl end. These data are confirmed by water accessibility determined by MD simulation. The results give important topological information on the hydrophobic binding cavity of  $\beta$ -LG. The calyx is large and hydrated at the entrance and becomes narrower and hydrophobic towards the bottom.

## 6.2 AGGREGATION OF MODEL PROTEINS

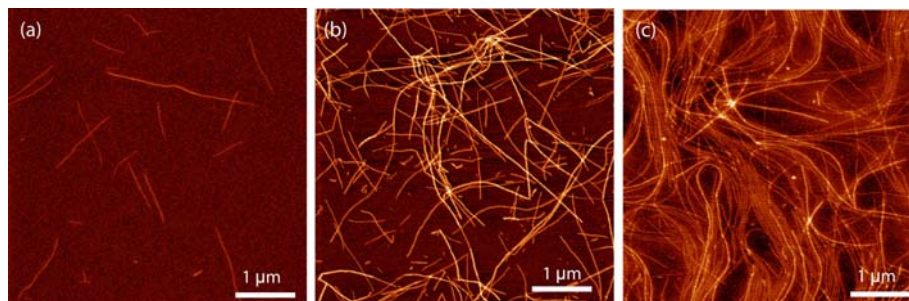
### 6.2.1 Fibrillar aggregation of $\beta$ -Lactoglobulin in the presence of copper ions

Amyloid aggregation of proteins in fibrillar structures, a phenomenon of fundamental importance in many neurodegenerative diseases, is also becoming a promising method for the self-assembly of nanostructured materials. Transition metal ions, which are commonly found in association with pathological amyloid plaques, are known to affect fibril morphology and growth rates, providing a handle to control their physical properties. We have studied the effect of the presence of copper ions on the fibrillation of  $\beta$ -lactoglobulin ( $\beta$ -LG), a model protein with distinctive aggregation properties. The process was investigated under conditions favoring the aggregation, i.e., at low pH and high temperature, by using several experimental techniques: Differential Scanning Calorimetry (DSC), Electron Paramagnetic Resonance (EPR), UV-Vis absorption spectroscopy and turbimetry, Atomic Force Microscopy (AFM).

The results indicate that the protein structure in solution is only slightly destabilized by the interaction with copper ions, as shown by DSC measurements. EPR spectroscopy evidences that the metal participates to the aggregation process without binding permanently to the protein. Non-monotonic variation in the absorbance of the protein solution as a function of the amount of copper ions reveals two competing processes, both affected by the presence of the metal: hydrolyzation of  $\beta$ -LG due to incubation at high temperature and low pH, and non-covalent association of the resulting protein fragment. Analysis of the AFM images shows that  $\beta$ -LG fibrils can have several distinct morphologies, corresponding to protofilaments and higher-order structures with increasing thicknesses. The presence of copper does not affect the aspect of the filaments but deeply increase

the rate of aggregation, as revealed by the surface density of the aggregates. Fibrillar aggregation proceeds through different processes: first nucleation of seeds, then fibril elongation and thickening into higher-order fibrils, possibly simultaneously with elongation.

The overall findings provide a comprehensive picture of the role of copper on the whole aggregation process of  $\beta$ -LG, ranging from protein conformational stability in solution to the kinetics of self-association and the morphology of the resulting fibrils.



**Fig. 3:** AFM images of fibrils obtained by heat-denaturation from (a) pure  $\beta$ -LG solution, (b)  $\beta$ -LG: $\text{Cu}^{2+}$  equimolar solution and (c)  $\beta$ -LG: $\text{Cu}^{2+}$  solution with 1:10 molar ratio. The height scale was 10 nm.

### 6.3 MOLECULAR DYNAMICS SIMULATION OF PROTEINS

#### 6.3.1 Binding mechanism for naturally-occurring and spin-labeled fatty acids in transport proteins

Molecular dynamics (MD) simulations have been used to study the anchoring of long-chain fatty acids to human serum albumin and  $\beta$ -lactoglobulin (Fig. 1). These two versatile proteins are able to bind, transport and deliver a variety of ligands that include drugs, metabolites and ions.

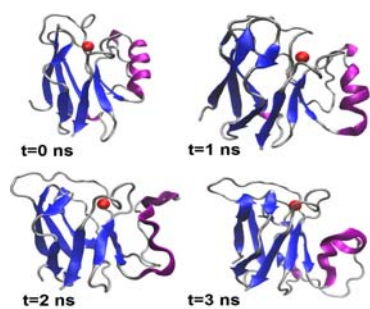
The association process was investigated for naturally-occurring fatty acids, such as palmitic and stearic acid. In these cases, *in silico* findings were compared with data reported by a variety of spectroscopic techniques. In addition, spin-labeled stearic acids containing a nitroxide group at five different positions along the acyl chain (*n*-SASL, *n*=5,7,10,12,16) were used. This allowed to probe the solvent accessibility into protein binding sites, and to combine the MD simulations with experimental data obtained by pulsed FT-EPR (Fourier-Transform Electron Paramagnetic Resonance) spectroscopy.

The overall results highlight how hydrophobic forces and specific electrostatic interactions with amino acid residues contribute to the uptake of fatty acids in proteins and demonstrate the effectiveness of computer simulations in complementing experimental techniques.

#### 6.3.2 Dynamical role of the metal binding loop in active site-engineered blue copper proteins

Molecular dynamics simulations have been carried out to investigate the inner motions of the blue copper native protein Azurin (Az) and of two Az active site-engineered mutants, to understand the role of the metal binding region in the protein dynamics. The copper ion in the active site of Az is coordinated by five ligands, three of which are encompassed in a 10-residue loop. This metal binding loop can be substituted with the corresponding region of other blue copper proteins, such as Amicyanin (Ami) and Plastocyanin (Pc), resulting in the two chimeric proteins AzAmi and AzPc, respectively. Both AzAmi and AzPc resemble Az in their overall structural conformation, whereas they are correspondingly similar to Ami and Pc in their spectroscopic and calorimetric features. Thus, differences in the dynamics of these three proteins is expected to be crucial to understand their physical properties.

The simulation results show that at room temperature the three proteins share the same secondary and tertiary structure. Principal component analysis indicates that residue motions are evident not only in poorly structured regions, but also in the metal binding loop and in the unique alpha-helix of Az. Therefore, cooperative inner motions coordinate distant regions across the whole protein structure.



*Fig. 2 – Snapshots of the unfolding process of Az at different simulation times.*

In addition, simulations at high temperature reveal that the early events in the unfolding process concern in each case the region of the alpha-helix that is the most distant from the metal binding loop. However, while in the three proteins the unfolding pathway is structurally similar, clear differences are found in the dynamics of specific regions that could contribute to explain experimental differences observed in their conformational stability.

## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2011**

1. R. Guzzi, M. Babalavi, R. Bartucci, L. Sportelli, M. Esmann, D. Marsh  
*Spin-echo EPR of Na,K-ATPase unfolding by urea*  
Biochim. Biophys. Acta – Biomembranes 1808 (2011) 1618–1628.
2. F. Scarpelli, R. Bartucci, L. Sportelli, R. Guzzi  
*Solvent effect on librational dynamics of spin-labelled haemoglobin by ED- and CW-EPR,*  
Eur. Biophys. J. 40 (2011) 273–279.
3. A. Stirpe, M. Pantusa, B. Rizzuti, L. Sportelli, R. Bartucci, R. Guzzi  
*Early stage aggregation and fibrillation of human serum albumin in the presence of metal ions*  
Int. J. Biol. Macromol. 49 (2011) 337–342.

#### **A.1.2 Publications on international journals accepted in 2011**

1. R. Guzzi, L. Sportelli, S. Yanagisawa, C. Li, D. Kostrz, C. Dennison  
*The influence of active site loop mutations on the thermal stability of azurin from Pseudomonas aeruginosa*  
Arch. Biochem. Biophys. accepted

#### **A.1.3 Publications on international journals submitted in 2011**

1. M. Pantusa, L. Sportelli, R. Bartucci  
*Resveratrol-HSA interaction. Influence of stearic acids bound to the protein.*  
Submitted to Biophys. Chem.
2. S. Evoli, R. Guzzi, B. Rizzuti  
*Dynamical role of the metal binding loop in active site-engineered blue copper proteins*  
Submitted to Proteins
3. B. Zappone, M. P. De Santo, C. Labate, B. Rizzuti, R. Guzzi  
*Catalytic activity of copper ions in the amyloid fibrillation of  $\beta$ -lactoglobulin*  
Submitted to Biomacromolecules
4. R. Guzzi, B. Rizzuti, R. Bartucci  
*Spin-labelled fatty acids interacting with  $\beta$ -lactoglobulin: evidences from EPR spectroscopy and Molecular Dynamics simulation*  
Submitted to J. Phys. Chem. B

## **B PUBLICATIONS ON BOOKS**

### **B.1 Invited contribution to Books in 2011**

1. R. Bartucci  
*Spin-Labeling EPR of Lipid Membranes*  
Long entry contribution to Encyclopedia of Biophysics, Springer-Verlag, Berlin-Heidelberg

## **C INVITED PRESENTATIONS**

### **C.1 Invited presentations at international conferences in 2011**

1. R. Bartucci  
*Pulsed FT-EPR studies of spin-labelled biosystems*  
Structure, function, folding and assembly of membrane proteins - Insight from Biophysics  
A Satellite conference of the 8<sup>th</sup> European Biophysics Congress, Tata (Ungheria), 27-31 August 2011

## **D PRESENTATIONS AT CONFERENCES**

### **D.1 Presentations at international conferences in 2011**

1. R. Guzzi, A. Stirpe, M. Pantusa, B. Rizzuti, L. Sportelli, R. Bartucci  
*Early stage aggregation of human serum albumin in the presence of metal ions*

Amyloid Fibrils Prions and Precursors: Molecules for Targeted Intervention, Halle (Germany), 25-28 August 2011

2. R. Guzzi, L. Sportelli, R. Bartucci  
*Electron spin echo studies of chain-labelled stearic acids interacting with  $\beta$ -lactoglobulin*  
8<sup>th</sup> European Biophysics Congress, Budapest (Hungary), 23-27 August 2011

## **D.2 Presentations at national conferences in 2011**

1. B. Rizzuti, R. Bartucci, L. Sportelli, R. Guzzi  
*Fatty acid association/dissociation in human serum albumin*  
SIF 2011– 97th National Congress of SIF (Società Italiana di Fisica), L'Aquila (Italy), 23-27 August 2011

## 7. PHYSICS AND APPLICATIONS OF THE SOFT MATTER

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Riccardo C. Barberi  
Enzo Cazzanelli  
Gabriella Cipparrone  
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Marco Castriota  
Melissa Infusino  
Gia Petriashvili  
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Clementina Provenzano  
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Ugo Cataldi  
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Raul Josuè Hernandez  
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Washington D.C. (*USA*)  
Bulgarian Academy of Sciences - Sofia (*Bulgaria*)  
Laboratory of Nanotechnology, UCLM (*Spain*)  
Moscow State University (*Russia*)  
Centre Paul Pascal - Bordeaux (*France*)  
University of Colorado - Boulder (*USA*)  
University of Tunis (*Tunisia*)

College de France - Paris (*France*)  
University of Marseille (*France*)  
University of Exeter (*UK*)  
Chalmers University - Goteborg (*Sweden*)  
University of Kent (*USA*)  
Polytechnic of Madrid (*Spain*)  
Polytechnic of Bucharest (*Romania*)  
University of Gent (*Belgium*)  
University of Ljubljana (*Slovenia*)  
Russian Academy of Sciences (*Russia*)  
University of Tblisi (*Georgia*)  
Philips Research Center (*The Netherlands*)  
Hewlett Packard Research Center (*UK*)  
University of Nizhny - Novgorod (*Russia*)  
University of California - Berkeley (*USA*)  
University of Nebraska (*USA*)  
University of Ohio (*USA*)  
University of Mexico–UNAM (*MEX*)  
European Synchrotron Radiation Facility (*France*)  
Rutherford Appleton Laboratory (*UK*)  
Stanford Synchrotron Radiation Laboratory (*USA*)  
University of Geneva (*Switzerland*)  
University of Verona (*Italy*)  
FBK Foundation of Trento (*Italy*)  
Università Politecnica delle Marche (*Italy*)  
University of Oxford (*UK*)  
Université Paris Diderot (*France*)

## Introduction

The research activity of the group will be devoted to the preparation and the characterisation of new soft materials, and to the study of their properties and of their interactions with external fields. The word soft matter, in our case is to be intended as partially disordered materials or, better, partially ordered fluids, with different properties depending on the length scale: polymers, liquid crystals, colloids, soft biological materials, in pure or mixed forms, and soft materials formed by, or including, nanoparticles. We will also study the interfaces of these materials with solid or fluid surfaces (organic-organic, organic-inorganic, biological-synthetic). Finally we will study the complex nature of these materials their complex interactions with electromagnetic and optical fields, as well as the complexity of systems in other related fields. Generally speaking the scientific interests of the group can be resumed as in the following:

### **7.1 MATERIALS, IN CLOSE COLLABORATION WITH CHEMIST GROUPS, BOTH FROM UNIVERSITY OF CALABRIA AND FROM OUTSIDE: NEW LIQUID CRYSTALS, COLLOIDAL SYSTEMS, NANOPARTICLES AND LIQUID CRYSTALS, POLYMERS, PHOTOPOLYMERS, BLENDING OF LIQUID CRYSTALS AND POLYMERS..... CHARACTERISATION (DIELECTRIC, RAMAN, ELLIPSOMETRY, ELECTRON MICROSCOPY...)**

#### **7.1.1 Spectroscopic Investigation On Innovative Materials**

The current research issues of the group concern spectroscopic investigation on innovative materials, in particular thin solid films, organic and inorganic, graphene and similar systems, polymers, liquid crystals and biological molecules. Finally, the group is interested to the micro-spectroscopic characterization of cultural heritage artifacts and mineralogical samples. Such activities are carried out in collaboration with other group, of our department, of other departments of our University and from outside, like the University of Verona and the FBK Foundation of Trento. For the year 2011 are worth of mention:

a) The micro-spectroscopic characterization of various materials entering in the assembling of POLYCRIPS (Polymer Liquid Crystal Polymer Slices), studied with the aim to obtain meta-materials when combined with gold nanoparticles. The liquid crystal E7 and the polymeric matrix NOA have been investigated, as well as the gold nano-particles coated by a thin layer of CTAB (Hexadecyltrimethylammonium bromide) and PINIPAM (Poly-N-isopropylacrylamide). Such investigation identified the liquid crystal vibration sensitive to the molecular orientation, so that a determination in situ of the liquid crystal orientation inside the POLYCRIPS was made. Moreover a reaction mechanism for the NOA polymerization has been suggested.

b) The micro-Raman study of graphene grown by CVD technique on Pt(111) surface, combined with other spectroscopic techniques, made in collaboration with another group of our department and one of University of Verona. The Raman analysis, together with the other techniques, reveal a good degree of order in the monolayer graphene grown on Pt(111), and the occurrence of two different orientations of the carbon domains with respect to the substrate; both generating a comparable Raman signal.

c) The continuation and extension of the study on the structural evolution of  $\text{WO}_3$  film grown by sol-gel technique on glass-ITO substrate, as a function of different thermal treatments, also carried out in collaboration with another group of our department.

d) In the field of systems with bio-medical applications, micro-Raman investigations have been carried out on ligand-receptor interaction for the protein GPR30 and for ligands like G1, 17- $\beta$  estradiol and similar ones.

e) In the field of application of our spectroscopic techniques to the cultural heritage, is remarkable the analysis of results of a micro-Raman investigation on a oil painting "Rebecca at the well", of Neapolitan anonymous, kindly provided by the MAON museum of Rende. The results have been presented to an international conference at Parma.

In addition, other studies have been carried out, also as thesis work of students:

*"Indagini chimico-fisiche su materiali cartacei invecchiati artificialmente"* Corso di Laurea in Scienze e Tecnologie per il Restauro e la Conservazione dei Beni Culturali (2011)

*"Indagini spettroscopiche micro-Raman sulle malte provenienti dal sito archeologico di Sassone"* Corso di Laurea in Tecnologie per il Restauro e la Conservazione dei Beni Culturali (2011)

### 7.1.2 Polymer-Liquid Crystal Phase-Separated Composites

By the method of photopolymerization-induced phase separation, thin single layers of LC-polymer composites were fabricated, having nematic (E7) droplets dispersed in the photopolymer NOA65. The nematic orientation in these layers was efficiently modified by rubbed Teflon nanolayer deposited on the cell substrates (ITO glass plate). Owing to the substrate treatment by Teflon, composite layers of well-ordered droplets and aligned nematic director in a single layer were obtained. The dispersion exhibits a nearly uniform distribution of the LC droplets, as well as a planar configuration of the nematic director. The LC-polymer composite single layers were characterized by the first-harmonic flexoelectro-optic spectra (the amplitude of transmitted light modulation versus the electric-field frequency). Sample prepared in a twisted cell was measured as varying the applied voltage and temperature. The peculiar minima (and their transformation and shift) observed in the spectra may be related mainly to the effect of the selective diffraction.

### 7.1.3 Chiral Liquid Crystals

Cholesteric liquid crystals (CLC) possess a self-organized supramolecular helicoidal periodic structure in which periodicity can be set from 100nm to infinity and which are also characterised by 100% selective reflection of circularly polarized light. CLCs can be used for several applications:

When a photoluminescent dye is hosted in a CLC matrix which has been prepared using nematic liquid crystals and chiral dopants, the dye acts as an active material in a resonator. Laser emission can therefore be obtained from the mixture when it is illuminated with a pump laser. The possibility to modify the helical pitch and then the photonic band gap structure of CLCs together with the possibility to exploit new luminescent materials with chiral properties allows to obtain mirrorless micro lasers with a finely tunable emission. We are also investigating lasing from liquid crystalline blue phases, that appear in short pitch cholesterics and have self-assembled three-dimensional cubic structures. The application of an electric field produces a versatile effect on the blue phases, causing a distortion of the cubic lattice and a consequent shift of the Bragg peaks. We are working to demonstrate that lasing in the blue phases may be tuned and easily controlled by an electric field and/or temperature and therefore be useful for photonic material based devices.

Generally, if a CLC is confined between two flat plates treated to provide boundary conditions with planar anchoring, the resulting texture is uniformly twisted everywhere and the helical axis is normal to the plates. When the distance  $d$  between the two boundary plates is small compared to the pitch  $p$  of the helix, then, these boundary conditions force the director throughout the sample to be perpendicular to the plates. In the narrow range of the confinement ratio  $C=d/p \approx 1$  of the thickness  $d$  over the equilibrium pitch  $p$ , one observes the formation of periodic gratings. When the boundary conditions of the confining plates is homeotropic one observes the formation of "bubbles". These bubbles are defects which form and grow after an external perturbation, but that can be stable in absence of the starting perturbation, and they have been observed for the first time in 1974 by Haas and Kawachi. The forming process of these exotic structures can be achieved by using three techniques: Applying a dc or low frequency voltage to the CLC cell, so that, an electrohydrodynamic turbulence is induced and the bubbles appear spontaneously after removal of the electric field; Raising the temperature of the CLC to the isotropic phase and then suddenly cooling it to room temperature; Applying a laser beam to the CLC cell. We investigate the formation and evolution of bubble domains with the goal to demonstrate that this kind of defects may hold a great interest due to their optical properties and that they can be used as an array of tunable micro-lenses.



#### 7.1.4 Titania Nanostructured Thin Films

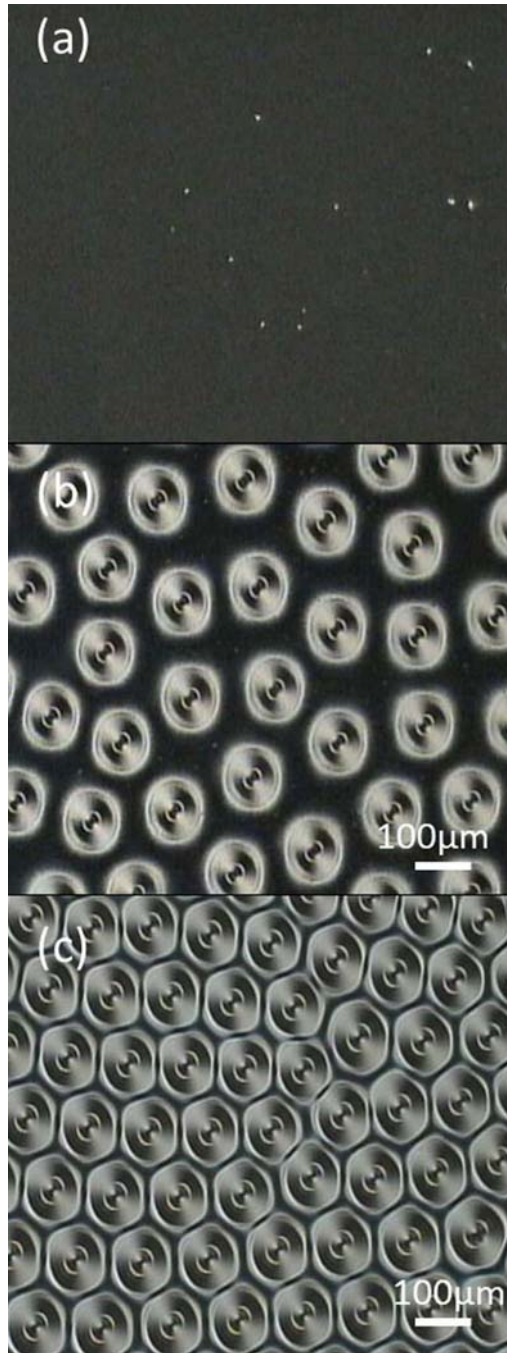
Since few year titania mesoporous and titania nanotubes are attracting the interest of a large number of researchers (Journal of Material Chemistry 17(2007)1451-1457) both for energy production (Nano Letters 6(2006)215-218, gas sensors (Thin Solid Films 496(2006)42-48) and for their interesting optical properties (Thin Solid Films 515(2006)2091-2096). Different procedures have been defined to produce ordered TiO<sub>2</sub> nanotube layer: by anodization of titanium foils (Journal of Material Science 42(2007)5539-5543, by sol gel synthesis (Macromolecules 41(2008)4551-4554) and by anodization of sputtered Ti films (Advanced Functional Materials 15(2005)1291-1296).

Our laboratory is involved in the study of TiO<sub>2</sub> nanotubes since two years during which a method to produce a homogeneous and transparent film of nanotubes on different type of substrates has been developed. During last year a method to fabricate titania nanotube arrays with anodization of Ti foils have been developed. Titanium foils (99,7% purity) with a thickness of 0,127 mm were used to cut out square specimens of 2,5 cm side. Before anodization specimens have been cleaned with ethanol, rinsed with de-ionized water and dried. Anodizations have taken place in a cell with conductive channel for electrolyte bath in vertical fashion, only one side of the specimen has been exposed to the bath with a surface of about 0,785 cm<sup>2</sup>.

To avoid process dependence on raising of gas, the platinum cathode has been positioned to leave gas to flow out from the cell.

An ethylene glycol bath with different ammonium fluoride concentrations ranging from 0,4 to 0,7 wt% and with H<sub>2</sub>O concentration ranging from 0 to 5% was used. Samples were anodized at 60 V for either 3 or 8 hours. To prevent cracking, fracturing and curling of specimens, after the anodization specimens were annealed at 470°C for 3h.

Anodizations have been carried out with good results regards to both neatness of data collected during processes and samples mechanical stability. However, a lot of work is still needed. Efforts are expected to complete samples characterization and insights are expected to relate nanotube arrays geometry to anodization parameters.

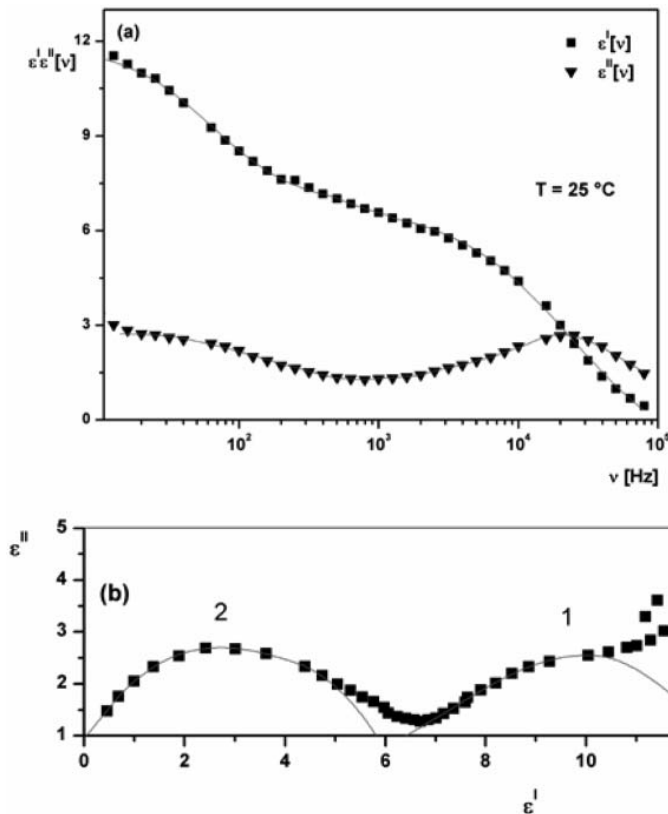


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CNC confined in homeotropic cell of 60 μm thickness observed under crossed polarizers: (a) virgin cell, nematic phase; (b) isotropic bubble distribution; (c) hexagonal bubble structure.

### 7.1.5 Dielectric Characterisation of an Orthoconic Antiferroelectric Liquid Crystal Mixture

Dielectric properties of the orthoconic smectic liquid crystalline mixture W-129, which presents both antiferroelectric and ferroelectric smectic C phases, have been studied in the frequency range from 10 mHz to 100 kHz in planar aligned cells. Some important relaxation modes were detected in SmCa\* and SmC\* phases. Dielectric increments, distribution parameters and relaxation frequencies of these modes have been evaluated at different temperatures. From the study of dielectric spectra a great variety of relaxation responses emerges that could indicate the presence of different SmCa\* subphases.



Dispersion and absorption curves (a) and Cole-Cole plot (b) of the dielectric spectra acquired for W-129 at 25°C. The solid red line shows the best theoretical fit of the Cole–Cole equation into experimental data.

## 7.2 SURFACES AND INTERFACES: CHARACTERISATION, INTERACTION LC-SURFACES, POLYMER SURFACES, ANCHORING, EFFECTS ON ELECTROOPTICS AND PHOTONICS

### 7.2.1 Nematic order Reconstruction as new tool to overcome topological barrier

Thermotropic Liquid Crystal (LC) molecules consist essentially of rigid core units with flexible side chains and they are usually represented by physicists as simple rods with cylindrical symmetry. Most of the LCs classical phenomena are described by the director  $\mathbf{n}$ , which indicates the average orientation of the calamitic molecules, and by an uniaxial scalar order parameter  $S$  that, in many cases, is considered mostly constant and independent of  $\mathbf{n}$ . Nevertheless, rich and intriguing physical phenomena in highly frustrated LC systems, such as topological defects, self organized colloidal dispersions in LC, LC emulsions, LC confined in porous materials or LC confined by means of topographic patterns can not be fully explained by this simplified classical description. In all these cases, a tensor order parameter  $\mathbf{Q}$ , which couples  $\mathbf{n}$  and  $S$ , needs to be defined, as pointed out by de Gennes.

For nematic LCs, the tensor description predicts two different ordered phases: uniaxial, which has a cylindrical symmetry with respect to the director, and biaxial, where such symmetry is broken and the system has two distinct optical axes. However, most nematogenic molecules are intrinsically biaxial even if they give rise to a uniaxial phase, which is usually a consequence of the rotational disorder around the long molecular axis. If, for instance, the rotational disorder is hampered, non-uniaxial features may appear and biaxial order could arise.

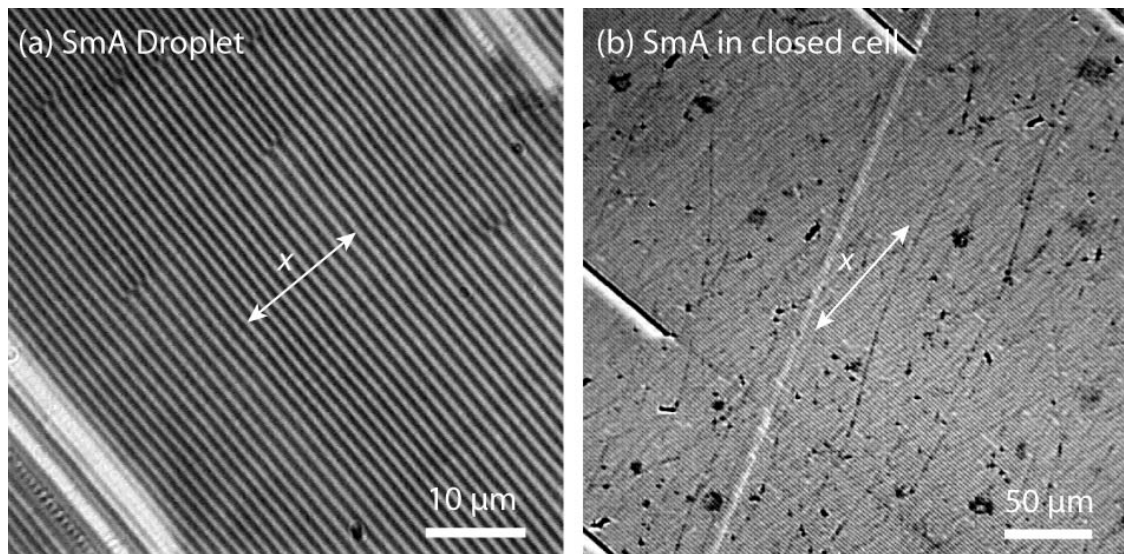
In this frame, in the last few years, we provided experimental investigations as well as theoretical foundation to the existence of biaxial domains within uniaxial LC systems, both in the bulk as well as at the LC interface. Recent experiments on LCs frustrated systems show that local and transient bulk biaxial order can be induced in calamitic nematics, and suggest that biaxiality should play a fundamental role in LC phenomena, which take place on nanometer scale. In particular, we proposed the biaxial order reconstruction in nematics as a new tool to describe locally transient biaxial states inside a uniaxial phase. This mechanism is capable to induce, for instance, by means of a strong electric field, a thin biaxial region, which connects two competing uniaxial nematic textures present in a symmetric  $\square$ -cell. We have also demonstrated that, the repulsive force between two surfaces confining a nematic topological defect can be influenced by biaxial states connecting competing alignments. All these phenomena are mathematically described by the eigenvalue exchange mechanism of the Landau de Gennes  $\mathbf{Q}$  order tensor formalism.

Moreover we have developed a new numerical model based on Finite Element Method to solve adequately the Landau de Gennes  $Q$  tensor model. The new method consists in a new adaptive grid techniques which moves dynamically the grid points of the mesh in the space where the gradient of the order and the local and transient biaxiality become important, keeping constant their connectivity and the number of mesh points inside the integration domain.

### 7.2.2 Ordered defect patterns in smectic liquid crystals

Linear arrays and bidimensional lattices of defects spontaneously appear in smectic-A liquid crystal (LC) films in response to incompatible anchoring conditions at the boundaries. Regular patterns can be easily observed in thin LC droplets deposited at the interface between a solid substrate that induces unidirectional parallel (planar) anchoring (e.g. a crystalline surface or a rubbed polymer film) and air that induces normal (homeotropic) anchoring. Linear arrays of "oily streak" defect domains are typically observed for film thickness smaller than 1  $\mu\text{m}$ , whereas quasi-hexagonal lattices of "focal conic domains" are observed for thicker films

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Linear arrays of oily streaks in thin smectic-A liquid crystal films.  $x$  is the planar anchoring direction. (a) Open film. (b) Closed cell between two glass plates

The formation of straight and parallel oily streaks appears to be a universal phenomenon that we could reproduce in thin open films (Fig. 1a) and closed cells (Fig. 1b) using various types of substrates and LCs. However, the inner structure of such domains is complex and depends on the details of the LC-substrate interaction [2]. Closed cells are particularly interesting from the point of view of applications as they allow to apply electric fields and change the features of the defect arrays.

Indeed, the most anticipated application of LC ordered patterns is as field-responsive templates (matrices, hosts) for guiding the spatial arrangement of nanoparticles (NP) such as nanospheres, nanorods or nanotubes, in regular arrays and lattices extending well beyond the size of a single. Working in collaboration with Emmanuelle Lacaze at the Institut de NanoScience de Paris (INSP) we have recently shown that gold NPs dispersed in the LC tend to segregate and remain trapped in linear defects forming long 'nano-chains' with a diameter comparable to the diameter of a single NP. When illuminated with polarized light, such nanochains show a polarization-dependent optical absorption due to the coupling of neighboring gold NPs in the plasmon resonance excited by a polarization parallel to the chain, whereas a perpendicular polarization produces the same optical response as for dispersed gold NPs.

### 7.2.3 Investigation and Applications of POLICRYPS Gratings

POLICRYPS is a structure made of perfectly aligned liquid crystal films separated by slices of almost pure polymer. Under suitable experimental and geometrical conditions, the structure is obtained by curing a homogeneous syrup of liquid crystal, monomer and curing agent molecules with a spatially modulated pattern of UV radiation. From an optical point of view, POLICRYPS is a holographic diffraction grating with a spatial periodicity that can be easily made of sub-micrometric scale, exhibiting diffraction efficiency values as high as 98%. Depending on the used substrate, the POLICRYPS grating can be utilized both in transmission or reflection,

with negligible scattering losses, and can be switched ON and OFF by application of an external electric field of the order of few V/ $\mu\text{m}$ . Concerning this structure, in the period of observation (2008), our interest has been devoted to the following arguments:

a) POLICRYPS gratings as switchable phase modulators

POLICRYPS gratings can be used as well as electrically controlled optical phase modulators. Arbitrarily polarized light normally incident on the structure experiences a birefringence that depends on the anisotropy of the composite liquid crystalline material and on the geometrical cell parameters. The sample behaves as a retardation plate in good agreement with the Jones matrix formalism. The birefringence of the modulator can also be tuned by applying a suitable voltage, while a negligible birefringence variation is detected by increasing the incidence power. This makes POLICRYPS structures suitable as switchable phase retarders for high power laser beams.

b) All-Optical switching in (1-2)D structures

We investigate high quality azo-POLICRYPS diffraction gratings to be used for fast all-optical switching in the visible range. The polymeric microstructures, produced in a multistep chemico-physical process, confine and stabilize a well aligned nematic liquid crystal (NLC) film, which is doped with a high performance mesogenic azobenzene dye, sensitive in the visible range. The all-optical switching of the grating between highly diffractive and transparent states is realized by a photochemical phase transition between nematic and isotropic phases based on the photoisomerization of azobenzene guest molecules. The effect, which is reversible and repeatable, is triggered by a visible pump irradiation and detected through the change in the diffraction efficiency of a low power probe light. Performances of the new structures are highlighted by investigating also the correlation between switching times and pump power.

#### **7.2.4 A Novel Polymer Matrix for Confinement and Alignment of Self-Organized Materials**

We report about the realization and characterization of a novel polymer matrix sculptured in photosensitive material devoted to micro/nano-confinement to stabilize a wide range of organic and biological components with self-arrangement properties at the nanoscale. The high quality morphology of a 2D polymer structure is obtained by combining a nano-precision level optical holographic setup and a multi-step chemical-physical process. The sharp and uniform morphology can be conveniently used as templates to be filled with high-refractive index materials or different soft composite elements. Due to their ability as self organization materials, short pitch cholesterics LC, azo dyes LC and ferroelectrics LC have been used. Various experimental studies have been carried out in order to investigate the efficiency of such structures for the realization of electro-optical and all-optical devices. Biological materials and DNA are currently under investigation.

#### **7.2.5 Realization and characterization of photonic aperiodic structures with a photo-polymerization technique**

These structures are realized using a novel approach to their fabrication based on the use of a programmable Spatial Light Modulator encoding Computer-Generated Holograms. This approach will also possibly allow (by comparison) a further understanding on the diffusion process driving the holographic realization of periodic structures such as diffraction gratings.

#### **7.2.6 POLICRYPS Gratings with metallic nano-inclusions towards Metamaterials**

Noble metal nanoparticles (NPs) exhibiting plasmonic properties attract wide interest in research for the possibility they offer to realize metamaterials. These have been predicted in 1969 by Veselago and they are materials that gain peculiar electromagnetic properties (e.g. negative refractive index) from their structure, rather than from their chemical composition. Thanks to recent advances in nanofabrication, first examples of such materials, which exhibit particular functionalities at optical frequencies, have been realized. However, the success of these results is limited by the typical size of devices that can be fabricated, which is actually very small (few square millimetres). Alternative approaches are emerging, which propose the use of self-assembling materials in order to overcome this issue and obtain the sought for greater structures, with less difficulty [Nanogold EU project, (2009-2012); Metachem EU project (2009-2013)]. An ambitious project is to combine metallic units with host materials whose dielectric properties can be tuned by an external control; indeed, a modification of the dielectric behavior of the host could correspond to a tuning action of the plasmon resonance frequency. In this regard, by combining the tunability of POLICRYPS structures with the plasmonic response of metallic NPs could give rise to novel metamaterial devices with tunable properties.

#### **7.2.7 Active Plasmonic systems realized in soft elastomers coated with gold NPs layers**

Soft elastomers are easy-to-fabricate cost-effective materials that are widely used in optofluidic, photonic and biomedical applications. Recently, we adopted these materials for realizing active plasmonic applications. In more detail, Au NPs have been layered on a polydimethylsiloxane (PDMS) substrate. There are several reasons why we chose such an approach. A first one is that an eventual device, being stretchable, should show tunable plasmonic features. Indeed, a stretching of the NP doped elastomer matrix should modify the relative distance between NPs and hence their electromagnetic coupling. Moreover, in case such prototype devices were successfully realized, its mass production should be straightforward: a master structure with the desired features would be easily replicated in the elastomeric support. This research line has been developed in collaboration with the group of Prof. Thomas Buerger of the University of Geneva.

### 7.2.8 Electrohydrodynamic Instabilities in Nematic Liquid Crystals

Anisotropic complex fluids, like e.g. liquid crystals, represent an interesting experimental example of a system exhibiting complex spatiotemporal behavior, a quite common feature in a wide range of systems far from equilibrium.

The early research in pattern formation focused on the presence of simple periodic structures, while the main questions currently addressed concern regimes characterized by higher complexity, that is, patterns that are more irregular in space and time. This is often related to the occurrence of intermediate states between order and turbulence. In particular, electro-hydrodynamic instabilities (EHD) in nematic liquid crystals (NLC) have been widely investigated by electro-optical experimental techniques. The occurrence of EHD is due to the molecular reorientation under the effect of an external electric field. A planar sample of NLC having a negative dielectric anisotropy can be driven through several regimes of increasing stochasticity by tuning the amplitude of the external field, and establishing a sequence of electro-hydrodynamic (EHD) instabilities. These are generated by the competition of two forces: a restoring dielectric torque, owing to the negative dielectric anisotropy, and a force exerted on the bulk fluid due to the charge separation produced by the positive conductivity anisotropy. As a result, a recurrent pattern of convective roll structures, associated to the periodic distortion of the director field,  $n(r)$ , are formed according with the model of Carr-Helfrich [1]. At low electric field's values a simple unidimensional distortion of the molecular field is observed. This regime, named Williams domains (WD), consists in a series of stationary convective rolls with periodicities of the order of the sample thickness. By increasing the amplitude of the electric field the convective cells are longitudinally stretched up to the formation of small scale spatial structures. This regime is indicated as Weak Turbulence (WT). For high values of the applied voltage WT pattern gives rise to the dynamical scattering mode (DSM1). Above a certain threshold of the applied voltage the DSM1 regime becomes metastable and shows a spontaneous transition towards a second DSM mode, this new regime is known as DSM2. This transition can be explained by a transient bimodal process.

We have investigated the spatiotemporal decorrelation processes in EHD turbulence. The scaling

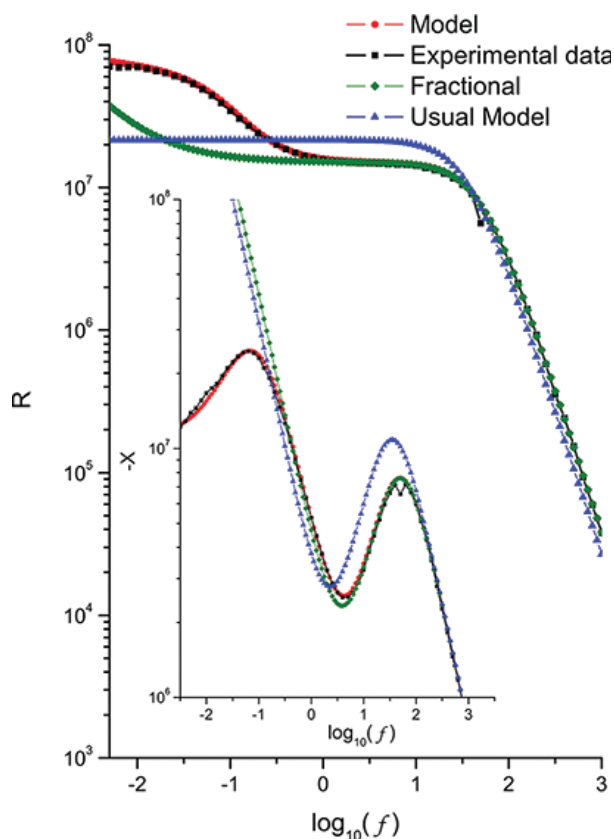
law  $\gamma \sim k^{-1}$  was found for the decorrelation rate in the perpendicular direction, suggesting a straining process resulting from fragmentation of large-scale structures. In the direction parallel to the large scale structures a

transition occurs at  $\epsilon = \epsilon_c \approx 3.5$ . At lower voltages we recover the scaling law  $\gamma \sim k^{-1}$  while at  $\epsilon > \epsilon_c$  an increasingly relevant role of the sweeping effect is recorded, and the scaling exponent approaches  $\mu \approx 1$  at higher voltages. Our conjecture on the role of decorrelation process provides an estimate of the characteristic random velocity  $u_0$ , responsible for the sweeping. The velocity linearly increases with  $V_0$ , with a slope change at  $\epsilon_c$ , in good agreement with independent direct measurements of the characteristic speed previously found in similar systems. The anisotropic crossover can be related to the transition from a weaker to a stronger turbulent regime in EHD. Finally, our results show that processes as the decorrelation properties of fluctuations, usually related to turbulent fluid flows, are universal.

We expect that other physical systems can share the same properties.

### 7.2.9 Dielectric Spectroscopy of Soft Matter

The electrical impedance data of different nematic liquid-crystal cells are analyzed in the framework of a model in which the diffusion of mobile ions in the bulk is governed by a fractional diffusion equation of distributed order. The boundary conditions at the electrodes limiting the sample are described by an integro-differential equation governing the kinetic at the interface that embodies, in particular, the usual kinetic equation for describing the adsorption-desorption process at the electrodes but is expressed in terms of a temporal kernel that can be chosen to cover scenarios that are not suitably described within the usual framework of blocking electrodes. The analysis is carried out by supposing that the positive and negative ions have the same mobility and that the electric potential profile across the sample satisfies the Poisson's equation. The results cover a rich variety of scenarios, including the ones connected to anomalous diffusion.



### 7.3 CONFINED SYSTEMS, NANOSCIENCES, PHOTONICS: LASING, GRATING, MEMORIES, HOLOGRAPHY, POLYCRIPS, SOLITONS

#### 7.3.1 Plasmonic Properties Of Core/Shell Metallic Nanoparticles (Nps) Dispersed In Solution

During 2011 the scientific research has been focused on the study of plasmonic properties of core/shell metallic nanoparticles (NPs) dispersed in solution. In particular we have performed an analysis on the coupling mechanisms between gain materials (organic dyes and quantum dots) and absorbing NPs, with the aim of compensate the optical losses. We focused our research principally on two dispersed systems, named "gain assisted" (in which dye is dispersed in solution) and "gain functionalized" (in which dye has been encapsulated into the silica shell). We performed measurements by means of a pump-probe set-up, through which it is possible to monitor the enhancement of Rayleigh scattering and transmission of a probe beam as a function of the pump energy. We have performed studies also on the alignment of liquid crystals molecules in plastic material (PDMS) in order to decrease the optical switching times; other theoretical and experimental studies have been conducted on the random laser emission in anisotropic complex fluids.

#### 7.3.2 Photosensitive organic materials

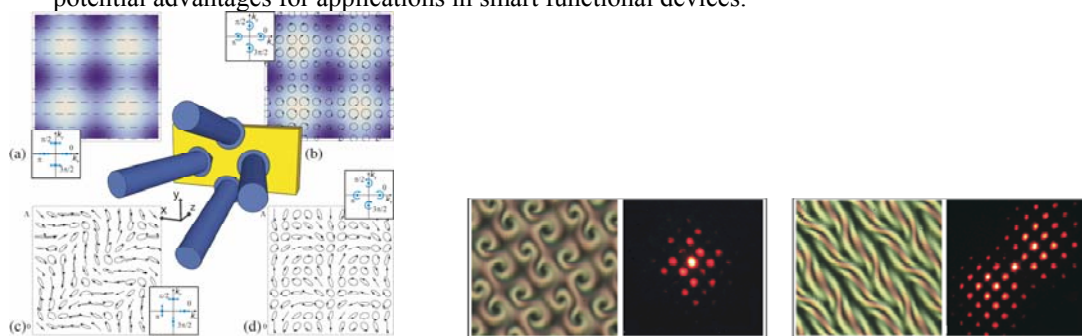
We investigated the photo-activated and photo-correlated properties of organic multifunctional molecular materials and their possible applications for photonic and optoelectronic devices. The attention to these materials, driven by their light-weight and by unique mechanical properties, as the prospect of manufacturing flexible and low-cost devices, is primarily due to the possibility to design molecules with properties tailored for specific applications, that can give rise to intermolecular interactions with high added value.

The organic materials are multifunctional polymers bearing three distinct functional groups, i.e. photosensitive azaromatic, photoconductive and chiral groups, directly linked to the side chain. The polymers possess, all at once, the three functionality that are the basis for optical storage based on induced modulation of the refractive index, chiro-optical switch, non-linear optical (NLO) and photorefractive and photoconductive applications. Although the aforementioned issues was the subject of intense study in recent years, their synergistic combination and their parallel presence in the materials have not yet been studied, and could lead to the observation of new phenomena. The polymers were supplied by the Chemistry Department of the Moscow State University,(Prof. V.

Shibaev) and Dipartimento di Chimica Industriale e dei Materiali, Università di Bologna (in the frame of the PRIN project “Synthesis and Functional Characterization of Photo-active Organic Semiconductors”).

### 7.3.3 Photoinduced optical anisotropies, holographic recording and supramolecular structuring

Supramolecular chiral periodic structuring of an amorphous azo-polymer has been demonstrated, exploiting the sensitivity of a polymer film to the light polarization. Selected 2D light patterns, coupled with the local and non-local material response to the optical field, permit the formation of spiral- and ribbon-like chiral structures. A four-beams holographic approach is adopted here in order to manage the intensity and the polarization of the writing light field in a bidimensional periodic fashion. The recorded structures are theoretically described by means of the Jones matrix method and experimentally investigated by microscope imaging and far field analysis, confirming the simultaneous occurrence of both linear and circular photo-induced anisotropies. Taking advantage of the unique characteristic of the polymer and of its response to light stimuli, we demonstrate the possibility of building optical architectures of great complexity in a very simple way. The results suggest an alternative approach to design new class of supramolecular chiral materials, characterized by high stability and complete reconfigurability, which have potential advantages for applications in smart functional devices.



### 7.3.4 Optical trapping and manipulation

The exploitation of optical forces represents at the same time a precise, non-invasive and gentle manipulation technique of micro and nano-particles. The most powerful and widely developed tool are the optical tweezers (OT) that have shown their tremendous potentiality for the manipulation without physical contact of systems with dimension ranging from tens of nanometers to hundreds of micrometers. The OT are applied in different research fields of the life sciences since they yield a non-invasive and near-infrared radiation. Moreover the advantages of remote control of micro and nano-particles and the sensitivity of the optical trap to piconewton-scale forces make OT an extremely useful tool also in the materials science and technology.

In the conventional approach, the optical forces and torques are mainly considered for the optical tweezers performances and the dynamics of the trapped particles, while the ambient fluid only yields a damping effect, through the viscous force. We have shown that a hydrodynamic force, known as Magnus force, can play an important role in the optical trapping and manipulation and should be considered whenever particles are forced to spin and dragged in a fluid, as well as shear and vortical flows are involved.

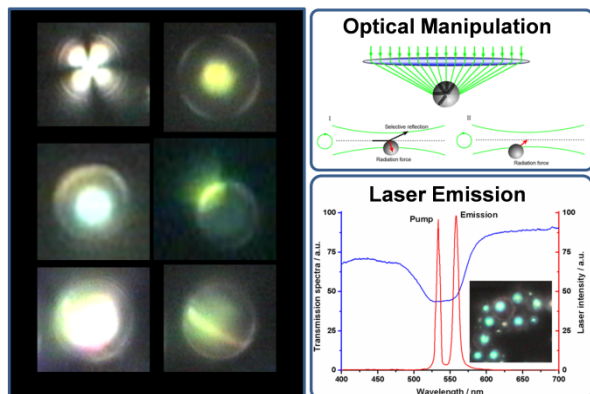
An ad hoc experiment has been designed based on a one-dimensional optical trap which carries angular momentum. The observed particle dynamics reveals the occurrence of this hydrodynamic force, which is neglected in the common approach. Its measured value is two orders of magnitude larger than the one predicted by the existing theoretical models for micrometric particles and low Reynolds number, suggesting the need for adequate modelling approach in case of optical micromanipulation and showing that the Magnus force can contribute to unconventional opto-hydrodynamic trapping and manipulation.

### 7.3.5 Microphotonic Devices for optical control and lasing

Micro and nanoscale particles are currently of great interest in the research areas of optical trapping and manipulations, microfluidics and optofluidics, sensors, photonics, colloids science and materials. Liquid crystals, for instance, represent an elegant example of such soft matter, as they are simple anisotropic fluids easy to manage but also rich in complexity, capable of self assembling in a variety of supramolecular arrangements and exhibit high response functions. We have developed a method for creating solid chiral microspheres exhibiting different internal helical configurations. The colloidal particles were obtained by using light-induced polymerization to harden cholesteric liquid crystal droplets. The polymerization process did not induce significant degradation of either the original helicoidal structures or the optical properties of the microparticles. In fact, the properties of the cholesteric droplets were fully preserved by the solid chiral microsphere. The ability to control the anchoring conditions at the LC-surrounding medium interface makes it possible to delineate how different internal



configurations within the cholesteric droplets could be obtained. The light-guided polymerization process let us to obtain solid chiral particles which, exhibit isotropic or anisotropic macroscopic properties depending on the internal geometry of the helicoidal structures. The choice of short and long pitches of cholesteric liquid crystal allowed us to identify the different kinds of self-organized cholesteric structures. Polarized optical microscopy was used to investigate the optical properties of the microspheres, while optical-tweezers experiments and laser emission from dye-doped microparticles were used to evaluate their unique features for applications in photonics, opto-fluidics, optical trapping among others at the microscopic scale.



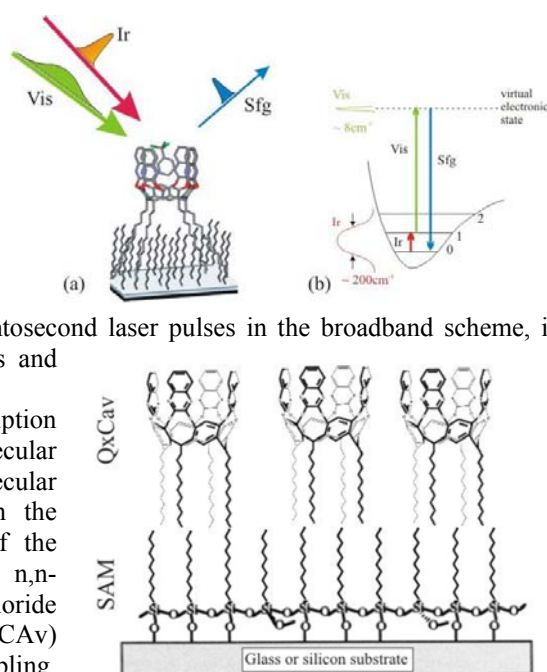
### 7.3.6 Nonlinear optical investigation of molecular recognition at interfaces for environmental and bio-chemical sensing

We explored the opportunities offered by nonlinear optics and, in particular, by the ultrafast sum-frequency generation vibrational spectroscopy (SFG-VS) in the fields of chemical and biochemical sensing. As a second-order nonlinear optical processes, SFG-VS has been proven to be a versatile analytical tool for non-invasive probing of any interface accessible by light, with intrinsic surface specificity, chemical selectivity and sub-monolayer sensitivity. With femtosecond laser pulses in the broadband scheme, it might permit the investigation of ultrafast surface dynamics and chemistry with sub-picosecond time resolution.

The SFG-VS has been used to provide a molecular-level description of surfactant-covered substrates and their hybrid bimolecular architectures with synthetic macrocyclic receptors. Molecular conformation and alignment have been deduced for both the surfactant and the synthetic receptor layer, as function of the material composition [i.e., n-octadecylsiloxane (OTS), n,n-dimethyl-n-octadecyl-3-aminopropyltrimethoxysilyl chloride (DMOAP), pyrazine- (PzCav) and quinoxaline-bridged (QxCav) cavitands] and deposition procedures [i.e., self-assembling, Langmuir-Blodgett, Langmuir-Schaefer].

Molecular-level evidence of the receptor-analyte complexation at the solid-gas interface has been obtained. DMOAP-PzCav and DMOAP-QxCav hybrid bilayers were exposed to vapor of acetonitrile. Unexpectedly, opposite orientation for the complexed analyte molecules has been found depending on the cavity depth.

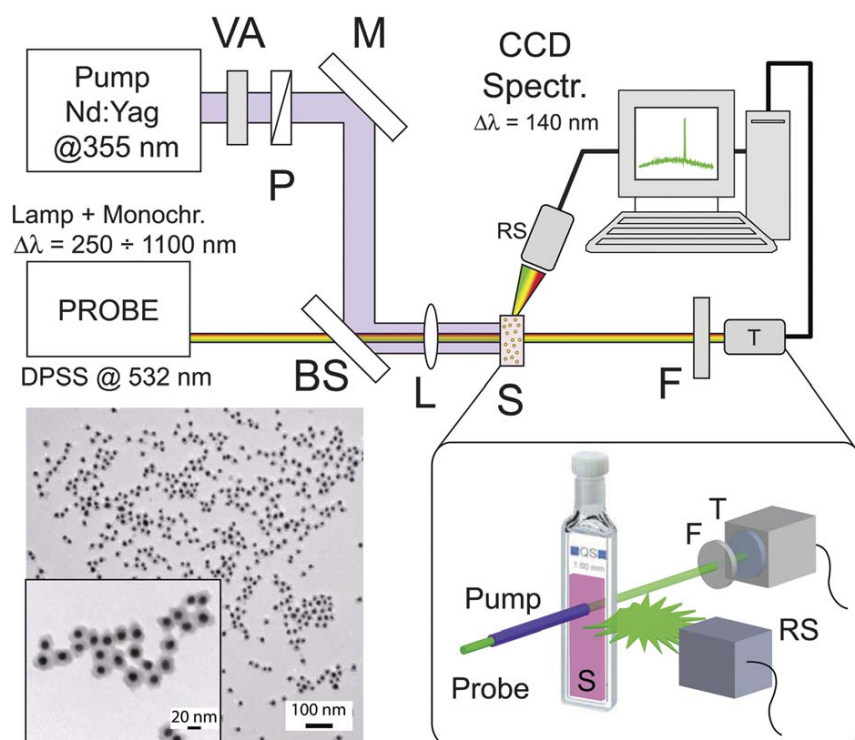
Membrane-mimetic architectures on solid substrates are extremely important for applications that include biosensor devices, preparation of biocompatible surfaces and fundamental studies of membranes. For biosensor applications, solid-supported membranes should contain both phospholipids and membrane receptors in their native conformation, be sufficiently rugged and have a high degree of stability, either in water or in air. Stabilized hybrid bilayer membranes (HBMs) have been obtained by Langmuir-Schaefer deposition of phospholipids on alkylsiloxane SAMs templates. Both OTS-DPPC and DMOAP-DPPC HBMs, supported on planar fused silica substrate, have been investigated by SFG-VS providing a description of their organization and structure.



### 7.3.7 Gain functionalized core-shell nanoparticles

We experimentally demonstrate that gain materials properly encapsulated into the shell surrounding metal nanoparticles (NPs) are responsible for the modification of the overall plasmon response of engineered

nanostructures. A comparison between designed systems based on functionalized core-shell NPs having different encapsulated dye molecules is presented. Experimental observations of Rayleigh scattering enhancement, accompanied by an increase of transmission as a function of gain, reveal striking optical loss compensation effects. Fluorescence lifetime measurements demonstrate a quenching of dye photoluminescence in functionalized core-shell NP samples with respect to pure dye solutions, confirming the strong resonant coupling occurring between the gain medium and gold NPs. Experimental evidence of a selective modification of the gain functionalized core-shell Au NP extinction curve is found, in good agreement with the results of a simplified theoretical model. The model verifies the causality principle through Kramers–Kronig dispersion relations for the investigated gain functionalized plasmonic nanostructure.



Pump-probe experimental set-up. VA: variable attenuator, P: polarizer, M: mirror, BS: beam splitter, L: lens, S: sample, F: filter, RS: Rayleigh scattering detector, T: transmission detector, DPSS: diodepumped solid state laser CW. TEM images of the obtained core-shell NPs with silica shell are shown at different scales for both Gf-C500 (inset at 20 nm scale) and Gf-DCM (100 nm scale) samples. The size of the metal core and the thickness of the silica shell were both measured by statistical analysis of TEM pictures.

#### 7.4 NANO-IMAGING OF BIOLOGICAL AND BIOCOMPATIBLE MATERIALS AND SURFACE FORCE APPARATUS (SFA)

##### Chromonic liquid crystals

The work concern the alignment of chromonic materials on different substrates. The difficult task is aligning them in homeotropic state, i.e. no optical birefringence is visible on polarized optical microscope and to avoid evaporation phenomena. We started studying the DSCG a well known chromonic material and then guanosine derivatives. We studied as well anticancer molecules and their aggregation by AFM varying solvent and substrates and their interaction with DNA.

##### 7.4.1 AFM and phase imaging on membranes

is used to provide a better insight in the topographical properties, on a scale not accessible to ESEM, of membranes developed at the Department of Chemical Engineering of Materials (UNICAL).

The chemical engineering group is developing membranes with ordered features made by block copolymers PS-PB (polystyrene and polybutadiene) changing the production conditions: solvents, temperature, presence of templates. The membranes are investigated in Tapping Mode AFM, with special attention to the 1<sup>st</sup> harmonic signal, to provide information on both their topographical and mechanical properties. The order in the surface morphology is correlated to the gas transport properties of the membranes. Membranes prepared using other materials are currently under investigation.

#### 7.4.2 Nano-imaging of biological materials

Advanced microscopy techniques, such as Atomic Force Microscopy (AFM) and Environmental Scanning Electron Microscopy (ESEM), are finding application in biology and biomedical investigations since they are non-destructive techniques and can be performed in liquid-humid environments.

AFM and ESEM are currently used to investigate the aggregation properties of proteins such as  $\beta$ -lactoglobulin as influenced by the presence of a substrate. This protein is used as a “model-protein” to study the different types of aggregation that can occur i.e. globular aggregates or fibrils formation. In particular the understanding of the mechanism of fibrils formation is important since it is related to several medical diseases (Alzheimer, Parkinson).

#### 7.4.3 Structural properties of hydrophobin aggregates revealed by atomic force spectroscopy in dynamic mode

Hydrophobins are small proteins (about 100 amino-acid residues) produced by fungi as soluble forms, self assembling into an amphipathic membrane when they reach an interface (e.g. medium-air or cell wall-air).

These proteins have been split in two groups, class I and class II hydrophobins, based on the differences in their hydrophobicity patterns, spacing of aminoacids between the cysteine residues and properties of the aggregates they form.

One distinguishing feature of class I hydrophobins is the characteristic rodlet structure observed on the hydrophobic side of an amphipathic protein film.

The interest in investigating such aggregates relies in the fact that their morphology and chemical-physical properties are reminiscent of amyloid fibrils, produced in mammals degenerative diseases; this similarity makes the hydrophobin rodlets a good model system.

We have investigated the protein *vmh2* class I hydrophobin from the fungus *pleurotus ostreatus* in order to obtain information about the structure of their assemblies, including monolayers, bilayers and aggregates under form of rodlets, with the motivation of a deeper understanding of the rodlets structure. We exploit force spectroscopy measurements in dynamic mode AFM to probe the wetting phenomenon of hydrophobin films and rodlets as a function of humidity on samples prepared by the Langmuir technique. We have demonstrated that the hydrophilicity of Langmuir-Schaefer film can be highlighted at the nanoscale by detecting the meniscus formation between the AFM tip and surface of the monolayer. On the other hand, we have demonstrated that no meniscus is formed, neither between tip and Langmuir-Blodgett monolayer, nor between tip and rodlets. These results confirm that the Langmuir-Schaefer monolayer is less hydrophobic than Langmuir-Blodgett one, as one would expect and as shown by contact angle measurements, but also demonstrate that it is less hydrophobic than rodlets. Moreover, by analyzing the phase versus distance curves performed in dry conditions for hydrophobin Langmuir-Blodgett film and rodlets, we have revealed the difference in the visco-elastic properties between Langmuir-Blodgett layers on one hand and Langmuir-Schaefer layers or rodlets on the other hand. This difference may be associated with the presence of the flexible loops that are exposed to the air in the Langmuir-Blodgett layer but interact with the substrate for Langmuir-Schaefer layer and with other molecules for rodlets. The interaction in rodlets at least partly occurs between two hydrophobins of the two layers in front of each other, as shown by the similarity between the hydrophilicity and visco-elasticity of hydrophobin bilayers and rodlets, measured by Atomic Force Spectroscopy. This similarity strongly suggests that rodlets are actually fragments of hydrophobic bilayer with molecular conformational changes with respect to simple superposed layers.

#### 7.4.4 Surface Force Apparatus

LICRYL owns the only Surface Force Apparatus (SFA) in Italy, that measures the normal force  $F$  between two macroscopic surfaces in gas or liquid. The distance  $D$  between the surfaces may be varied and controlled with sub-nm resolution from several microns to zero. To measure  $D$ , we use a multiple-beam optical interferometric technique based on fringes of equal chromatic order (FECO), which also allows to determine the refractive index  $n$  (sensitivity  $\pm 0.01$ ), the geometry of surface contact, and possible damage caused by loading and/or shearing. A series of springs and precision actuators allows to move the surfaces and measure  $F$  with a precision better than  $10^{-7}$  N.

The surfaces used in the SFA are composed of flexible transparent sheets of mica that are silvered on the outer face for optical interferometry and glued onto crossed cylindrical lenses. Other materials can also be used, including polymers and glass. The surfaces can be further modified *in situ* by adsorption of surfactants or polymers, with plasma treatment or through vacuum deposition to vary the physical-chemical properties of the surfaces, such as adhesion energy, hydrophobicity, roughness, wear-resistance, etc. At LiCryL, SFA is used to study liquid crystals confined to nanometric geometries, where they undergo uncommon structural transitions due to the strong influence of surface anchoring and biaxiality. In addition, SFA will be used to study long, flexible and strongly hydrated biopolymers, which show lubricating and wear properties in aqueous solution and could have important biomedical applications in the cure of arthritic diseases of the articular cartilage

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*Broad band tuning of the plasmonic resonance of Gold nanoparticles hosted in self-organized soft materials*,  
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*Optical interrogation system based on holographic soft matter filter*,  
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Nature Photonics, 5, 234-238(2011)
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*Universal Soft Matter Template For Photonic Applications*,  
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*Separation of Information on Amplitude, Absolute Phase and Polarization in Young's Interference Experiment*,  
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*Separation of Information on Intensity, Absolute Phase and Polarization in Pattern Formation by the Superposition of Slightly Inclined Electromagnetic Beams*,  
MOLECULAR CRYSTALS AND LIQUID CRYSTALS, 549, 113-119 (2011)
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*PEG-templated mesoporous silica nanoparticles exclusively target cancer cells*,  
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- Pucci, Daniela; Pasini, Paolo; Versace, Carlo,  
*Special Issue: Proceedings of the 5th Italian-Japanese Workshop on Liquid Crystals 2010 (JILC2010) and the 9th Italian National Meeting on Liquid Crystals (SILC2010) Preface,*  
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#### A.1.2 Publications on international journals accepted in 2011

- F. Ciuchi, A. Mazzulla, N. Scaramuzza, E. K. Lenzi, L. R. Evangelista,  
*Fractional Diffusion Equation and the Electrical Impedance: Experimental Evidence in Liquid-Crystalline Cells,*  
to appear on J. Phys. Chem. C 2012.
- Y.G. Marinov, G.B. Hadjichristov, S. Marino, L. Todorova<sup>1</sup>, S. D'Elia, C. Versace, N. Scaramuzza, A.G. Petrov  
*Flexoelectro-Optical Behaviour of Layers Formed by Polymer-Liquid Crystal Phase-Separated Composites,*  
to appear on Bulg. J. Phys. (2012)
- Antonio De Luca, Melanie Ferrie, Serge Ravaine, Massimo La Deda, Melissa Infusino, Alireza R. Rashed,  
Alessandro Veltri, Ashod Aradian, Nicola Scaramuzza, Giuseppe Strangi,  
*Gain functionalized core-shell nanoparticles: the way to selectively compensate absorptive losses,*  
to appear on J. Mater. Chem. (2012)
- L. Marino, E. Bruno, M. P. De Santo, F. Ciuchi, S. Marino, N. Scaramuzza,  
*Dielectric Characterisation of an Orthoconic Antiferroelectric Liquid Crystal Mixture,*  
to appear on Mol. Cryst. Liq. Cryst. (2012)

### B PUBLICATIONS ON CONFERENCE PROCEEDINGS

#### B.1 Publications on international conference proceedings in 2011

- L. De Sio; R. Caputo; U. Cataldi; J. Dintinger; H. Sellame; T. Scharf; C. Umeton ,  
*Metallic subentities embedded in micro-periodic composite structure,*  
Proc. SPIE 8145, DOI: 10.1117/12.892777 (2011)
- C. Umeton; L. De Sio; R. Caputo; S. Ferjani, G. Strangi, and R. Bartolino,  
*Universal soft matter template: from photonic to metamaterial applications,*  
Proceedings of SPIE, Vol. 8114, DOI: 10.1117/12.892781 (2011)
- A. E. Vasdekis, J. Cuennet, L. De Sio, and D. Psaltis,  
*Optofluidics based on liquid crystal microflows,*  
Proceedings of SPIE, Vol. 8114, DOI: 10.1117/12.893277 (2011)
- A. E. Vasdekis, J. Cuennet, L. De Sio, and D. Psaltis,  
*Integrated optofluidic modulators based on nematogen flows,*  
in CLEO:2011 - Laser Applications to Photonic Applications, OSA Technical Digest (CD) (Optical Society of America, 2011), paper CTuZ6. ”

### C INVITED PRESENTATIONS

#### C.1 Invited presentations at international conferences in 2010

- 10<sup>th</sup> Workshop “NOVEL OPTICAL MATERIALS AND APPLICATIONS”, Cetraro, Italy  
Title: *Realization and characterization of light sculptured structures including liquid crystals and doped with metal nanoparticles*  
Authors: R. Caputo, L. De Sio, C. Umeton
- NANOGOLD Dissemination Workshop, Lausanne, Switzerland (2011).  
Title: *Self-organization of liquid crystal phases doped with metal nanoparticles in periodical polymeric structures,*  
Authors: R. Caputo, L. De Sio, U. Cataldi, C. Umeton.
- 14th International Topical Meeting on Optics of Liquid Crystals, Yerevan, Armenia (2011)  
Title: *POLICRYPS: from gratings to metamaterials*  
Authors: C. Umeton

4. SPIE Optics + Photonics 2011, San Diego, USA  
 Title: *Universal soft matter template: from photonic to metamaterial applications*  
 Authors: C. Umeton; L. De Sio; R. Caputo; S. Ferjani, G. Strangi, and R. Bartolino

## D PRESENTATIONS AT CONFERENCES

### D.1 Presentations at international conferences in 2011

1. (2011) *5th International Congress on Advanced Electromagnetic Materials in Microwaves and Optics - Metamaterials 2011*, October 10th - 15th, Barcellona, (Spain)  
**Oral:** *Gain assisted and gain functionalized core-shell nanoparticles: A multi-pronged approach to compensate loss in metamaterials*,  
 A. De Luca, M. Infusino, I. Pastoriza-Santos, M. Grzelczak, L. Curri, M. Striccoli, G. Strangi  
  
**Poster:** *Plasmonic nanoparticles self-organization in chiral liquid crystals*,  
 M. Infusino, A. De Luca, A. Rahimi Rashed, N. Scaramuzza, G. Strangi, R. Bartolino
2. (2011) *Science at IPCF - In onore del Prof. G. Parisi - Medaglia Max Planck - 13 April* (Rome)  
**Oral:** *Gain induced transparency in optical metamaterials*  
 A. De Luca, G. Strangi, M. Infusino, R. Bartolino
3. P. Pagliusi, C. Provenzano, A. Mazzulla, G. Cipparrone,  
*Liquid crystal polarization gratings allow for artifact-free circular dichroism measurements*,  
 European Conference on Liquid Crystals ECLC-2011, Maribor (SL), February 6-11 (2011)
4. P. Pagliusi, C. Provenzano, V.P. Shibaev, G. Cipparrone.  
*Polarization holograms in amorphous polymer with photoinduced linear and circular birefringence*,  
 European Conference on Liquid Crystals ECLC-2011, Maribor (SL), February 6-11 (2011)
5. P. Pagliusi, C. Provenzano, E. Lepera, A. Mazzulla and G. Cipparrone,  
*Artifact-free and real-time chiroptical measurements by polarization gratings*,  
 Mediterranean Workshop and Topical Meeting “Novel Optical Materials and Applications” NOMA 2011, Cetraro (IT), June 5-10, (2011)
6. P. Pagliusi, E. Lepera, C. Provenzano, A. Mazzulla, G. Cipparrone,  
*Polarization gratings allow for real-time and artifact-free circular dichroism measurements*,  
 SPIE Microtechnologies, Prague (CZ), April 18-21 (2011).
7. G. Cipparrone, R. J. Hernandez, P. Pagliusi, C. Provenzano,  
*Exploring unconventional capabilities of holographic tweezers* (invited),  
 SPIE Optics and Optoelectronics, Prague (CZ), April 18-21 (2011).
8. R.J. Hernandez, P. Pagliusi, C. Provenzano and G. Cipparrone,  
*Exploring opto-hydrodynamic capabilities of optical tweezers*,  
 27) COST Action MP0604 “Optical Micro-Manipulation by Nonlinear Nanophotonics”, Cetraro (IT), June 8-10 (2011)
9. G. Cipparrone,  
*Polarized optical tweezers and liquid crystal droplets: new insights on micromanipulation and hydrodynamics*,  
 (invited),  
 Optics of Liquid Crystal Conference 2011, Armenia (Yerevan)
10. R. Caputo, B.J. Tang, L. De Sio, G. H. Mehl and C. Umeton,  
*Policryps assisted self-organization of Nematic Gold Nanoparticles*,  
 14th International Topical Meeting on Optics of Liquid Crystals, Yerevan, Armenia (2011)
11. L. De Sio; R. Caputo; U. Cataldi; J. Dintinger; H. Sellame; T. Scharf; C. Umeton  
*Metallic subentities embedded in micro-periodic composite structure*,  
 SPIE Optics + Photonics 2011, San Diego, USA
12. R. Caputo, L. De Sio, J. Dintinger, H. Sellame, T. Scharf and C.P. Umeton



*Plasmonic Response in POLICRYPS-like Structures including Metallic Subentities*,  
11th European Conference on Liquid Crystals, Maribor, Slovenia (2011)

13. M. Castriota, E. Cazzanelli, A. Fasanella, R.G. Agostino T. Caruso and A. Policicchio,  
*Raman Scattering Enhancement Associated to Sodium Oxide Formation after Thermal Treatment of Glass Substrates*,  
17/05 – 19/05/11 “XX CONGRESSO NAZIONALE A.I.V. -Energia e materiali: Tecnologie a confronto e prospettive”, Padova, Italy.
14. A. Fasanella, K. Cosentino, A. Beneduci, G. Chidichimo, E. Cazzanelli and M. Castriota,  
*Thermal structural evolutions of dimyristoylphosphatidylcholine (DMPC) - water systems investigated by micro-Raman Spectroscopy*,  
17/05 – 19/05/11 “XX CONGRESSO NAZIONALE A.I.V. -Energia e materiali: Tecnologie a confronto e prospettive”, Padova, Italy.
15. M. Castriota, A. Fasanella, E.Cazzanelli, L. De Sio, R. Caputo and C. Umeton,  
*E7 liquid crystal molecular orientation in POLICRYPS holographic lattice: a micro-Raman spectroscopic analysis*,  
**05/06 – 11/06/2011** “NOMA 2011, 10<sup>th</sup> Mediterranean Workshop and Topical Meeting” “Novel Optical Materials and Applications”, Cetraro, Italy.
16. A. Fasanella, M. Castriota, E.Cazzanelli, L. De Sio, R. Caputo and C. Umeton,  
*Orientation of Liquid crystal director in POLICRYPS systems determined by micro-Raman spectroscopy*,  
**03/07 – 10/07/2011** “International School of Liquid Crystals, 18<sup>th</sup> Course “Liquid crystal nanostructures and self-assembling: from organic electronics to metamaterials” and “2<sup>nd</sup> School of Italian Liquid Crystal Society , Erice, Italy.
17. E. Platania, E. Cazzanelli, G. De Santo, A. Fasanella and M. Castriota,  
*Micro-spectroscopic Raman investigation on the canvas oil painting “Rebecca at the well”, of Neapolitan anonymous*,  
05/09 – 08/09/11 “6<sup>th</sup> International Congress on the application of Raman Spectroscopy in Art and Archaeology”, Parma, Italy.

## OTHER PRESENTATIONS AND EVENTS

Progetto di Grande Rilevanza Scientifica Italia-Messico 2011-2013, finanziato dal MAE.

Beside the basic scientific research, the year 2011 has been devoted to the technology transfer activity, planned in the enterprise project NOTREDAME, include in the general university project CRESCITA (Conoscenza Ricerca e Sviluppo per l'avvio in Calabria di Imprese a Tecnologia Avanzata) proposed by the “PARCO SCIENTIFICO E TECNOLOGICO DELLA CALABRIA-CALPARK”.

Within such activity, is worth mentioning, beside an Italian patent, the following achievements:

- a) Winning the prize “Cervelli in movimento (Brains in motion), 2011” offered by Bridges to Italy, in collaboration with Tech Coast Angels, the University of California Irvine and TECHNEST , the institution of Università della Calabria to help innovative enterprises.
- b) Receiving a citation by the newspaper “America Oggi”: Page 2, 09 October 2011, concerning the technological transfer project NOTREDAME (iNnOvative substrates Development for electro-opticAl polyMeric flexible self consistent devices for applications in the field of the Energy saving).
- c) Finalist, among 2139 participants, in the “Working Capital 2011-Premio Nazionale Innovazione” sponsored by Telecom Italia and by Associazione degli Incubatori Universitari Italiani (PNI).

## 8. SURFACE ELECTRON SPECTROSCOPY (SPES)

### *Professors and Researchers*

Elio Colavita (Group Leader)  
Gennaro Chiarello  
Raffaele Giuseppe Agostino  
Vincenzo Formoso  
Tommaso Caruso

### *Postdoc fellows*

Enrico Maccallini  
Alfonso Policicchio  
Antonio Politano

### *PhD students*

Antonio Marino  
Myrsini Antoniou  
Marco Caputo

### *Technicians*

Salvatore Abate (Lycril/CNR)  
Giovanni Desiderio (Lycril/CNR)  
Vito Fabio  
Eugenio Li Preti

### *Collaborators*

Benedek (*Università Milano-Bicocca, Italy*)  
D. Fariás (*Universidad Autonoma de Madrid, Spain*)  
R. Miranda (*IMDEA Nanociencia, Madrid, Spain*)  
F. de Juan (*Berkeley National Laboratory, Usa*)  
V. Alzari (*University of Sassari, Italy*)  
C. Esposito Corcione (*University of Salento, Italy*)  
L. Peponi (*Instituto de Ciencia y Tecnologia de Polimeros, Madrid, Spain*)  
V. Nazarov (*Academia Sinica, Taipei, Taiwan*)  
E. Chulkov (*Universidad Pais Vasco, Spain*)  
V. Silkin (*Donostia International Physics Center, San Sebastian, Spain*)  
A. Goldoni (*Elettra, Trieste, Italy*)  
G. Mariotto (*University of Verona, Italy*)  
P. Milani (*University of Milano, Italy*)  
P. Rudolf (*Material Science Center, University of Groningen, The Netherlands*)  
C.E. Bottani (*Politecnico of Milan, Italy*)  
J. bNagy (*Dept of chemical and material engineering, Univ. of Calabria*)  
G. Golemme (*Dept of chemical and material engineering, Univ. of Calabria*)  
S. La Rosa (*Elettra, Trieste, Italy*)  
S. Scalese (*CNR, Catalina, Italy*)  
D. Gournis (*University of Ioannina, Greece*)  
F. Alamgir (*Brookhaven National Laboratory, New York, USA*)  
G. Froudakis (*University of Crete, Greece*)  
P. Trikalitis (*University of Crete, Greece*)  
F. Alamgir (*Georgia Institute of Technology, Atlanta, Georgia, USA*)  
G. Valenti (*University of Bari, Italy*)

### **Awards**

Dr. Antonio Politano, post-doc fellow from September 1<sup>st</sup>, 2011, received the “**Alfredo di Braccio**” Award by **Accademia Nazionale dei Lincei** as the best Italian researcher in Physics under 35 years.

### **Research subjects:**

#### **8.1 CHEMISORPTION ON METAL SURFACES**

8.1.1 Vibrational investigation of catalyst surfaces: Change of the adsorption site of CO molecules upon coadsorption

8.1.2 The adsorption and co-adsorption of oxygen and carbon monoxide on Pt<sub>3</sub>Ni(111)

8.1.3 Carbon monoxide interaction with oxygenated nickel single-crystal surfaces

## 8.2 GRAPHENE/METAL INTERFACES

8.2.1 Water interaction with quasi-freestanding graphene

8.2.2 Dispersion and Damping Processes of  $\pi$  Plasmon in Monolayer Graphene on Pt(111)

8.2.3 Evidence of Kohn anomalies in quasi-freestanding graphene on Pt(111)

8.2.4 Phonon dispersion of quasi-freestanding graphene on Pt(111)

8.2.5 Evidence for acoustic-like plasmons on epitaxial graphene on Pt(111)

## 8.3 SPECTROSCOPIC AND MICROSCOPIC STUDIES OF CARBON AND METAL-OXIDE NANOSTRUCURES

8.3.1 Microscopic wetting and bundling of TiO<sub>2</sub> Hierarchical Nanostructures.

8.3.2 ZnTPP dye adsorption on nanostructured TiO<sub>2</sub>.

### Introduction

Chemisorption on metal surfaces and graphene / metal interfaces have been one of the goals of the research group. Adsorption on solid surfaces and the individuation of adsorption sites for reactive chemical species are both important to tailor catalytic properties of surfaces and interfaces. Vibrational spectroscopy has been used for individuating adsorption sites in coadsorption systems on catalyst surfaces. The same high-resolution technique has been used to study the  $\pi$  plasmon in a monolayer of graphene grown on Pt(111) and its interaction with water. The eSEM microscope has been used to study wetting by water and successive drying of TiO<sub>2</sub> layers deposited by pulsed laser deposition. The bundling of these structures induced by wetting and successive drying, has been observed in real time. We saw the final formation of a micrometer-size pattern with statistically uniform islands separated by channels. An international patent was published and several proposals were written. It also happened that the group leader did not publish any scientific work during the year

## 8.1 CHEMISORPTION ON METAL SURFACES

### 8.1.1 Vibrational investigation of catalyst surfaces: Change of the adsorption site of CO molecules upon coadsorption

The understanding of the elementary steps occurring in catalytic reactions in the heterogeneous phase is one of the foremost goals of surface science. Adsorption on solid surfaces is the first step in catalytic reactions. Therefore, the individuation of adsorption sites for reactive chemical species is essential information to tailor catalytic properties of surfaces and interfaces. As a matter of fact, the change in adsorption site often implies a different reactivity for chemisorbed adsorbates and a selective catalytic activity. We have evidenced how vibrational spectroscopy can be used for individuating adsorption sites in coadsorption systems on catalyst surfaces. In particular, we studied CO coadsorption with oxygen, nitrogen, and hydrogen on the Ni(111) and the Ni(100) surfaces. Our attention was focused on the determination of CO adsorption sites in the various investigated systems. For CO adsorbed alone on the substrate, the preferential adsorption sites are the 3-fold hollow on the (111) face and the atop and bridge for the (100) surface. Striking changes in the CO adsorption site occur whenever CO is coadsorbed with other chemical species. In the CO + O coadsorption system, atop sites are populated by CO on the Ni(111) surface, while bridge and 4-fold hollow sites are occupied on Ni(100). In the CO + N phase on Ni(111), CO molecules occupy the bridge site of the pseudo-(100) reconstructed surface. For a H-precovered Ni(100) surface at 150 K, the C-O stretching frequency is near its gas-phase value, thus suggesting the occurrence of a weakly bonded CO phase without changes of adsorption sites.

### 8.1.2 The adsorption and co-adsorption of oxygen and carbon monoxide on Pt<sub>3</sub>Ni(111)

High-resolution electron energy loss spectroscopy has been used to investigate the adsorption and co-adsorption of oxygen and CO on the Pt<sub>3</sub>Ni(111) surface. For the sake of comparison, similar measurements have also been performed on the Pt(111) surface. We find that CO adsorbs at the same manner on both surfaces. By contrast, significant differences between the two surfaces exist concerning the adsorption of O and the co-adsorption of O with CO.

### 8.1.3 Carbon monoxide interaction with oxygenated nickel single-crystal surfaces

High-resolution electron energy loss spectroscopy has been used to study the coadsorption of CO and O on Ni(111) and Ni(100) surfaces at 250 K. These vibrational measurements showed that with increasing surface coverage at 250 K, the preadsorbed O caused changes in the adsorption sites for the after-adsorbed CO molecules revealing, however, dissimilar adsite alterations for the two Ni single crystals. Also, a different behavior towards carbonate formation was found upon CO adsorption at 250 K on Ni(100) and Ni(111) surfaces precovered with O at 250 K.

## 8.2 GRAPHENE/METAL INTERFACES

### 8.2.1 Water interaction with quasi-freestanding graphene

Vibrational spectroscopy has been used to study the interaction of water with quasi-freestanding graphene grown on Pt(111). A sharp O-H (O-D) vibrational band centered at 457 (337) meV is a direct evidence of the existence of non-H- (non-D-) bonded water molecules at the water/graphene interface. This finding is expected to play a significant role in understanding the behavior of water at hydrophobic surfaces. Such finding is in agreement with results reported for water adsorbed on other hydrophobic surfaces and with the behavior of water confined in carbon nanotubes and between graphene sheets.

Loss measurements also show that water molecules dosed at room temperature can dissociate giving rise to C-H bonds. The formation of the C-H bonds strongly attenuates the optical phonons of the graphene sheet. On the other hand, at 100 K water has been found to adsorb only in molecular state. Present findings should be taken into account in engineering graphene-based devices which should work at atmospheric pressure and at room temperature

### 8.2.2 Dispersion and Damping Processes of $\pi$ Plasmon in Monolayer Graphene on Pt(111)

High-resolution electron energy-loss spectroscopy has been used to study the  $\pi$  plasmon in monolayer graphene grown on Pt(111). A quadratic dispersion has been observed, in contrast to the linear dispersion reported for monolayer graphene grown on SiC(0001) and in agreement with recent experiments on graphene/Ni(111). Despite the weak interaction of the monolayer graphene with the Pt(111) surface, our results indicate that the screening by the underlying metal substrate strongly influences both the dispersion relation and the damping processes of the plasmon mode of  $\pi$  electrons.

### 8.2.3 Evidence of Kohn anomalies in quasi-freestanding graphene on Pt(111)

High-resolution electron energy loss spectroscopy has been used to probe phonon dispersion in quasi-freestanding graphene epitaxially grown on Pt(111). We report direct evidence of the existence of Kohn anomalies in the  $\Gamma$ - $E_{2g}$  and  $K$ - $A_1'$  optical phonon modes. These findings contrast with previous results on graphene/Ni(111), for which no Kohn anomalies were detected. Thus, such dissimilarity arises from the different interactions existing between graphene/Pt(111) (quasi-freestanding graphene) and graphene/Ni(111) (strongly interacting with the substrate). Hence, the phonon spectrum can be used to finely study the graphene-substrate coupling.

### 8.2.4 Phonon dispersion of quasi-freestanding graphene on Pt(111)

High-resolution electron energy loss spectroscopy has been used to probe phonon dispersion in quasi-freestanding graphene epitaxially grown on Pt(111). Loss spectra clearly show different dispersing features related to both acoustic and optical phonons. Results have been compared with graphene systems which strongly interact with the substrate, i.e. the nearly-flat monolayer graphene (MLG)/Ni(111) and the corrugated MLG/Ru(0001). We found that the phonon dispersion of graphene/Pt(111) reproduces well the behavior of pristine graphite. This could be taken as an indication of the negligible interaction between the graphene sheet and the underlying Pt substrate. The softening of out-of-plane modes observed for interacting graphene/metal interfaces does not occur for the nearly-free-standing graphene/Pt(111).

### 8.2.5 Evidence for acoustic-like plasmons on epitaxial graphene on Pt(111)

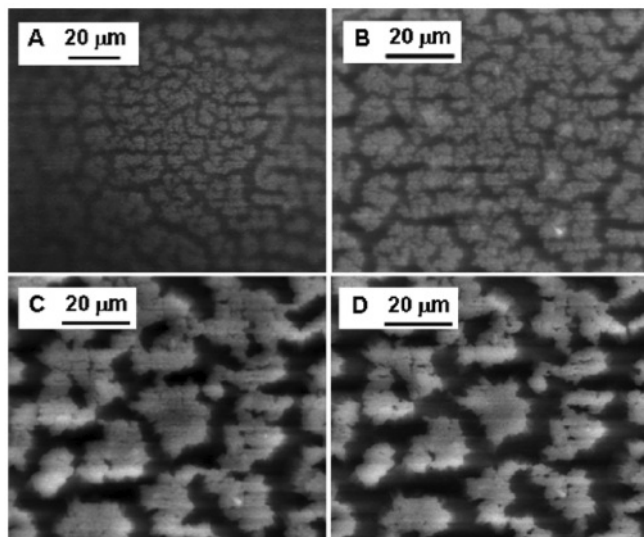
The dispersion and the damping of the sheet plasmon in a graphene monolayer grown on Pt(111) have been studied by using angle-resolved electron energy loss spectroscopy. We found that the dispersion relation of the plasmon mode confined in the graphene sheet is linear, as a consequence of the screening by the metal substrate. Present results demonstrate that the presence of an underlying metal substrate could have striking consequences on the plasmon propagation even in the case of a system which exhibits a weak graphene-substrate interaction. Moreover, we found that Landau damping essentially occurs via interband excitations starting above the Fermi wave vector. On the contrary, intraband transitions do not have a significant influence on the collective mode.

## 8.3 SPECTROSCOPIC AND MICROSCOPIC STUDIES OF CARBON AND METAL-OXIDE NANOSTRUCURES

### 8.3.1 Microscopic wetting and bundling of $TiO_2$ Hierarchical Nanostructures

Environmental Scanning Electron Microscopy (eSEM) is capable to perform microscopic studies of films in “real life” conditions (temperatures range  $-10^{\circ}C \div 50^{\circ}C$ , pressures up to 80mbar) and to observe wetting and drying phenomema at micro and nano metric length scales. We have used the eSEM to study wetting by water (increasing water pressure until condensation occurs on the cold films) and successive drying of  $TiO_2$  layers deposited by pulsed laser deposition. The

TiO<sub>2</sub> films were produced at the Politecnico di Milano (NanoLab) and were characterized by vertically oriented, columnar-like structures. It was possible to observe in real time the bundling of these structures induced by wetting and successive drying, and the final formation of a micrometer-size pattern with statistically uniform islands separated by channels. The eSEM investigations have supported the description of this phenomenon, due to capillary forces acting between the columns during evaporation of the water layer. This structure is interesting for those applications where wettability, high specific surface area, and porosity at different length scales are needed at the same time (e.g., photocatalysis, photoelectrochemical cells, or cell growth studies just to mention some).



eSEM images of a TiO<sub>2</sub> PLD film (40 Pa O<sub>2</sub>, thickness 10 μm) as (A) water floods the surface at 7.70 mbar, and as water pressure is reduced after completewetting at pressure > 7.80 mbar: (B) 7.40, (C) 7.30, and (D) 7.20 mbar."

### 8.3.2 ZnTPP dye adsorption on nanostructured TiO<sub>2</sub>

In the field of dye sensitized solar cells (DSSC), based on a nanostructured TiO<sub>2</sub> anode as proposed by M. Graetzel in 1991, the research is still focused on the basic mechanisms involved in the photocurrent production with the aim of further increasing the cell efficiency. Among the factors that determine the efficiency of DSSC, the interaction between the dye molecules and the TiO<sub>2</sub> surface is still under investigation. In order to elucidate the formation mechanisms and the properties of the TiO<sub>2</sub>-dye molecule interface, photoelectron spectroscopies have been employed exploiting their high surface sensitivity. However, most of the work has been carried out on TiO<sub>2</sub> single crystals, while in a standard DSSC, the TiO<sub>2</sub> anode consists of titania nanostructures. To this respect studies on dye adsorption on controlled titania nanostructures are needed in order to understand parameters affecting a dye molecule adsorption on a nanostructured material.

The adsorption of Zn-tetra phenyl porphyrin (Zn-TPP) molecules on TiO<sub>2</sub> films synthesized by pulsed laser deposition was studied by synchrotron radiation experiments (Material Science and Bach beamlines at Elettra).

In particular, the molecules' electronic structure and the bonding with the substrate were analysed by core level and valence band photoemission and x-ray absorption spectroscopy. While valence band resonant photoemission at N 1s and C 1s level permitted to study the charge transfer between ZnTPP and TiO<sub>2</sub>.

The results show that both the bonding and the charge transfer are strongly influenced by the substrate preparation procedures. On the pristine TiO<sub>2</sub> surfaces (mainly showing anatase structure and fully stoichiometric) the Zn-TPP monolayer bonding is done via carbon atoms of the phenyl rings. Instead, defects made on the TiO<sub>2</sub> substrate induce a different bonding, via carbon atoms of the Zn-TPP macrocycle. The resonant photoemission at the C edge is influenced by this behaviour (see figure), and charge transfer between phenyl rings and substrate is quenched when a Zn-TPP monolayer is grown on pristine and fully oxidized TiO<sub>2</sub> films.

## INTERNATIONAL PATENT

1. D. Gournis, P. Trikalitis, G. Froudakis, R.G. Agostino,  
*Functional nanoporous materials for gas storage applications*,  
International Patent n. PCT WO20119889A2,  
published on 27/01/2011

## INTERNATIONAL AND NATIONAL PROJECTS

1. Proposal full title:  
"INNOX - INNovative OXide hierarchical nanostructures for advanced energy and sensing applications"  
Italian FIRB - PROGRAMMA "FUTURO IN RICERCA" project  
Name of the coordinating person: Dr. A. Li Bassi  
List of participants:  
1 (Coordinator) Politecnico di Milano  
2 Dipartimento di Fisica, Università della Calabria,  
3. Istituto Nanoscienze, Consiglio Nazionale delle Ricerche  
4 ISTITUTO DI ACUSTICA E SENSORISTICA "ORSO MARIO CORBINO", Consiglio Nazionale delle Ricerche  
Application in 2011

## A PUBLICATIONS ON SCIENTIFIC JOURNALS

### A.1 Publications on international journals

#### A.1.1 Publications on international journals printed in 2011

1. Politano, A., Marino, A.R., Formoso, V., Chiarello, G.  
*Water adsorption on graphenePt(111) at room temperature: A vibrational investigation*  
AIP Advances 1 (4) , 042130 (2011)
2. Politano, A., Marino, A.R., Formoso, V., Chiarello, G.  
*Hydrogen bonding at the water/quasi-freestanding graphene interface*  
Carbon 49 (15) , pp. 5180-5184 (2011)
3. Politano, A., Chiarello, G.  
*Vibrational investigation of catalyst surfaces: Change of the adsorption site of CO molecules upon coadsorption*  
Journal of Physical Chemistry C 115 (28) , pp. 13541-13553 (2011)
4. Politano, A., Borca, B., Hinarejos, J.J., Vázquez De Parga, A.L., Fariás, D., Miranda, R.  
*Helium reflectivity and Debye temperature of graphene grown epitaxially on Ru(0001)*  
Physical Review B - Condensed Matter and Materials Physics 84 (3) , 035450 (2011)
5. Politano, A., Marino, A.R., Formoso, V., Fariás, D., Miranda, R., Chiarello, G.  
*Evidence for acoustic-like plasmons on epitaxial graphene on Pt(111)*  
Physical Review B - Condensed Matter and Materials Physics 84 (3) , 033401 (2011)
6. Chiarello, G., Marino, A.R., Formoso, V., Politano, A.  
*The adsorption and co-adsorption of oxygen and carbon monoxide on Pt<sub>3</sub>Ni(111): A vibrational study*  
Journal of Chemical Physics 134 (22) , 224705 (2011)
7. Politano, A., Chiarello, G.  
*Carbon monoxide interaction with oxygenated nickel single-crystal surfaces studied by vibrational spectroscopy*  
Vibrational Spectroscopy 55 (2) , pp. 295-299 (2011)
8. Fusi M., Maccallini E., Caruso T., Casari C., Li Bassi A., Bottani C., Rudolf P., Prince K.C., Agostino R.G.,  
*Surface electronic and structural properties of nanostructured titanium oxide grown by pulsed laser deposition*  
Surface Science, 605 (2011) 333–340

9. M. Fusi, F. Di Fonzo, C. S. Casari, E. Maccallini, T. Caruso, R. G. Agostino, C. E. Bottani and A. Li Bassi, *Island Organization of TiO<sub>2</sub> Hierarchical Nanostructures Induced by Surface Wetting and Drying* Langmuir 2011, 27(5), 1935–1941.

#### A.1.2 Publications on international journals accepted in 2011

1. Politano, A., Marino, A.R., Chiarello, G.  
*Phonon dispersion of quasi-freestanding  $\beta$  rapheme on Pt(111)*  
to appear on Journal of Physics Condensed Matter (2012)
2. Politano, A., Marino, A.R., Formoso, V., Chiarello, G.  
*Evidence of Kohn anomalies in quasi-freestanding graphene on Pt(1 1 1)*  
to appear on Carbon (2012)
3. Politano, A., Marino, A.R., Formoso, V., Farias, D., Miranda, R., Chiarello, G.  
*Quadratic Dispersion and Damping Processes of  $\pi$  Plasmon in Monolayer Graphene on Pt(111)*  
Plasmonics, doi:10.1007/s11468-011-9317-1
4. Politano, A., Chiarello G.  
*Influence of electron quantum confinement on the electronic response of metal/metal interfaces*  
to appear on Reviews in Plasmonics (2012)
5. Díaz, C., Politano, A., Martín, F., Farias, D., Miranda, R.  
*He, Ne and Ar scattering from Ru(0001)*  
to appear on Journal of Physics Condensed Matter (2012)

## 9. THEORETICAL PARTICLE PHYSICS AND APPLICATIONS

### *Professors and Researchers*

Roberto Fiore  
Domenico Giuliano  
Alessandro Papa  
Marco Rossi

### *Postdoc fellows*

Francesco Caporale

### *PhD students*

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Gennaro Cortese (XXIV cycle)  
Gabriele Infusino (XXIII cycle)  
Beatrice Murdaca (XXV cycle)  
Amedeo Perri (XXVI cycle)

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V.S. Fadin (*Budker Institute for Nuclear Physics, Novosibirsk, Russia*)  
S. Fazio (*Brookhaven National Laboratory*)  
D. Fioravanti (*Università di Bologna & INFN-Bologna, Italy*)  
P. Giudice (*University of Swansea*)  
A.V. Grabovsky (*Budker Institute for Nuclear Physics, Novosibirsk, Russia*)  
M. Gravina (*University of Cyprus*)  
P. Grinza (*Universidad de Santiago de Compostela, Spain*)  
D.Yu. Ivanov (*Sobolev Institute of Mathematics, Novosibirsk, Russia*)  
L.L. Jenkovszky (*Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine*)  
A. Lavorini (*Università della Calabria, Italy*)  
V. Magas (*Universidad de Barcelona, Spain*)  
M. Mancini (*Università di Perugia & INFN-Perugia, Italy*)  
D. Rossini (*Scuola Normale Superiore, Pisa, Italy*)  
F. Sanfilippo (*Université de Paris Sud, Orsay, France*)  
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A. Trombettoni (*SISSA-Trieste, Italy*)  
V.R. Zoller (*ITEP, Moscow, Russia*)

## **Introduction**

The research activity during the AA 2010-11 included the following subjects:

- phenomenology of hadron collisions and Quantum Chromodynamics (QCD) in the high-energy limit;
- non-perturbative properties of gauge theories discretized on a space-time lattice;
- field theory of correlated devices;
- integrability in the N=4 supersymmetric Yang-Mills theory.

A major part of this activity has been carried on in collaboration with other research groups in Italy and abroad. For the part concerning the non-perturbative study of gauge theories on a space-time lattice, a large use has been done of the PC farm “Majorana” of the Istituto Nazionale di Fisica Nucleare (INFN) – Gruppo Collegato di Cosenza, hosted by the Physics Department.

## **9.1 QCD IN THE HIGH-ENERGY LIMIT AND HADRON PHENOMENOLOGY**

### **9.1.1 QCD in the high-energy limit**



We have studied the connection between complete representations of gauge invariant operators and their Möbius representations acting in a limited space of functions. The possibility to restore the complete representations from Möbius forms in the coordinate space is proven and a method of restoration is worked out. The operators for transition from the standard BFKL kernel to the quasi-conformal one have been found both in Möbius and total representations.

We have studied the process proton-proton to jet1- jet2-X, where the jets have large transverse momenta and are produced in high-energy proton-proton collisions with a large rapidity gap between them. In this case the (calculable) hard part of the reaction receives large higher order corrections proportional to logarithms of the center-of-mass energy, which can be accounted for in the BFKL approach. Specifically, we have calculated in the next-to-leading order the vertex (impact-factor) for the inclusive production of the jet. We have compared our results for the vertex with the former calculation by Bartels et al. and, in the case of the quark contribution, clarified the discrepancy present in the literature. A paper has been issued on the arXiv, which has been submitted for publication.

The next-to-leading order jet vertex has been calculated also in the small-cone angle approximation, which turns to be very useful for a numerical analysis of the double differential cross section for the production of Mueller-Navelet jets in proton-proton collisions. The related paper is ready and will appear soon.

We have studied the process proton-proton to h1- h2-X, where the identified hadrons h1 and h2 have large transverse momenta and are produced in high-energy proton-proton collisions with a large rapidity gap between them. In this case the (calculable) hard part of the reaction receives large higher order corrections proportional to logarithms of the center-of-mass energy, which can be accounted for in the BFKL approach. Specifically, we have described in the next-to-leading order the calculation of the vertex (impact-factor) for the inclusive production of the identified hadron. The related paper is ready and will appear soon.

### 9.1.2 Hadron Phenomenology

The top-bottom weak current generates strong left-right asymmetry of neutrino-nucleon interactions at ultra-high energies. We have separated contributions of different helicity states and make use of the k-factorization to derive simple and practically useful formulas for the left-handed and right-handed components of the conventional structure function  $2xF_3 = F_L - F_R$  in terms of the integrated gluon density. We have shown that  $F_L \gg F_R$  and, consequently,  $xF_3 \approx F_T$ . The structure function  $F_2 = F_S + F_T$  at  $Q^2 \ll m_i^2$  appears to be dominated by its scalar component  $F_S$  and the hierarchy  $F_S \gg F_L \gg F_R$  arises naturally. We have evaluated the total neutrino-nucleon cross section at ultra-high energies within the color dipole BFKL formalism.

Currently available estimates of the gluon-fusion effect in ultra-high energy neutrino-nucleon interactions as well as in DIS on protons suffer from uncertainty in defining the scattering profile function  $\Gamma(b)$ . Indeed, the area  $S$ , in the impact parameter space populated with interacting gluons varies by a factor of 4 - 5 from one analysis to another. To get rid of uncertainties we specify the dipole-nucleon partial-wave amplitude  $\Gamma(b)$ , which meets the restrictions imposed by both the total dipole-nucleon cross section and the small angle elastic scattering amplitude. The area  $S$  becomes a well defined quantity proportional to the diffraction cone slope. We have solved numerically the non-linear color dipole BFKL equation and evaluate the UHE neutrino-nucleon total cross section. Our finding is that the saturation is a rather weak effect, less than about 25%, up to  $E_\nu \sim 10^{12}$  GeV.

Exclusive diffractive production of real photons and vector mesons in electron-proton collisions has been studied at HERA in a wide kinematic range. We have presented a Regge-type model of real photon production (Deeply Virtual Compton Scattering), as well as production of vector mesons (VMP) treated on the same footing by using an extension of a factorized Regge-pole model proposed earlier. The model has been fitted to the HERA data. Despite the very small number of the free parameters, the model gives a satisfactory description of the experimental data, both for the total cross section as a function of the photon virtuality  $Q^2$  or the energy  $W$  in the center of mass of the  $\gamma^*p$  system, and the differential cross sections as a function of the squared four-momentum transfer  $t$  with fixed  $Q^2$  and  $W$ .

## 9.2 LATTICE GAUGE THEORIES

### 9.2.1 Finite density QCD

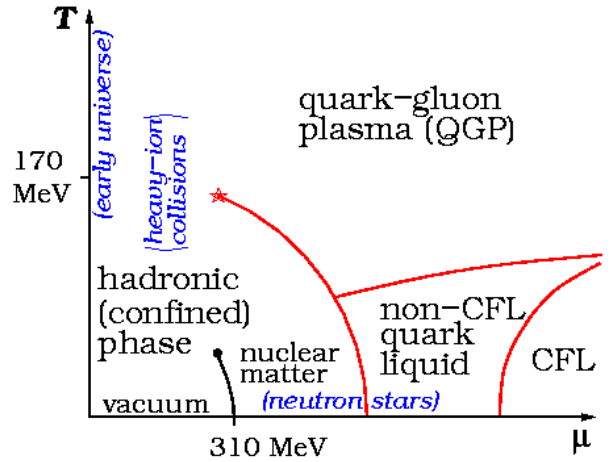
We have revisited the determination of the pseudo-critical line of QCD with two degenerate quarks at non-zero temperature and baryon density or isospin density by the method of analytic continuation. We have determined the pseudo-critical couplings at imaginary chemical potentials by high-statistics Monte Carlo simulations and revealed deviations from the simple quadratic dependence on the chemical potential visible in earlier works on the same subject. Finally, we have studied the implications of our findings for the shape of the pseudo-critical line at real chemical potential, comparing different possible extrapolations. Moreover, we have studied the order of the transitions in the

region of small temperature and high density and near the so-called Roberge-Weiss point at imaginary chemical potential.

**Figura 1: QCD phase diagram on the baryon chemical potential - temperature plane.**

### 9.2.2 Berezinsky-Kosterlitz-Thouless (BKT) phase transitions in spin models

We have studied the phase transitions in the 2D  $Z(N)$  spin vector model, for  $N > 4$ . Renormalization group arguments support the scenario with three phases: high-temperature (or massive), BKT (or massless), low-temperature (ordered), separated by two BKT transitions. We have investigated both analytically and numerically the renormalization group equations, established the position of the critical points of the two phase transitions and computed the critical index  $\nu$ . For  $N=7, 17$  the critical points have been located by Monte Carlo simulations and some of the corresponding critical indices have been determined.



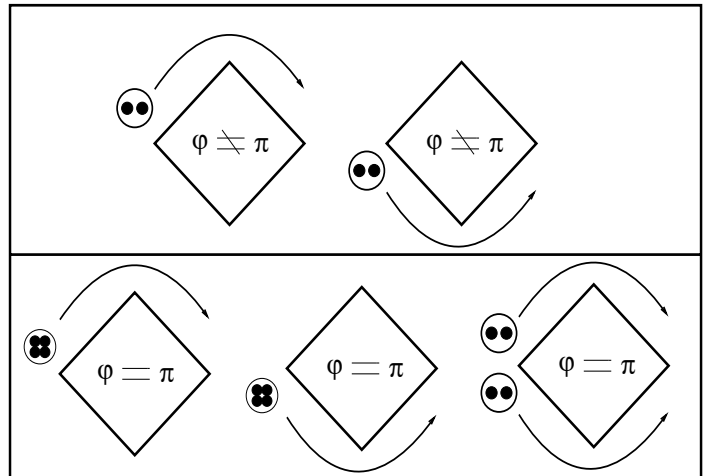
### 9.2.3 Planar QED in external fields

We have investigated planar Quantum ElectroDynamics (QED) with two degenerate staggered fermions in an external magnetic field on the lattice. Our results indicate that there is dynamical generation of mass for two-dimensional massless Dirac fermions in the weak coupling region. This has some implications on the quantum Hall effect in graphene.

## 9.3 FIELD THEORY OF CORRELATED DEVICES

### 9.3.1 Theory of quantum-coherent Josephson devices

Using boundary field theory formalism to describe the phases accessible to a tetrahedral qubit coupled to Josephson junction chains acting as Tomonaga-Luttinger liquid leads, it has been shown that, pertinently tuning the fabrication and control parameters, it is possible to stabilize an interacting phase corresponding to an attractive finite coupling fixed point of the phase diagram. Such a stable phase is characterized by the emergence of a quantum doublet which is robust against the noise in the external control parameters (magnetic flux, gate voltage), as well as against the decoherence induced by the coupling of the tetrahedral qubit with the superconducting leads. Finally, a protocol has been provided, to read and to manipulate the state of the emerging quantum doublet, and it has been argued how a tetrahedral Josephson junction network operating near the new finite coupling fixed point may be fabricated with today's technologies.



**Figura 2: (Top) Tunneling of a single Cooper pair across an impurity in a Josephson network; (bottom) coherent tunneling of pairs of Cooper pairs across the same device.**

### 9.3.2 Strong coupling, spin-1/2 representation of the one-dimensional Bose-Hubbard model

A rigorous mapping of the one-dimensional Bose-Hubbard Hamiltonian one-dimensional the spin-1/2 XXZ Hamiltonian has been derived, which is valid for Hubbard  $U$  finite, though larger than the single-boson hopping, provided the parameters of the XXZ-Hamiltonian are properly chosen. In particular, this allowed to express the correlation functions of single-boson operators of the Bose-Hubbard model in terms of correlation functions of spin operators in the XXZ model.

This gave rise to the possibility of “simulating” spin-spin correlation within the XXZ-model in terms of the correlation functions of a model with tunable parameters (the Bose-Hubbard model). As a side result, it is expected to be possible to use the derived correspondence to simulating the physics of impurities in antiferromagnetic chains (Spin-Kondo effect) within the one-species BH model.

## **9.4 FIELD THEORY OF HYBRID DEVICES**

### **9.4.1 Josephson effect in a normal electronic chain connected to two superconductors**

An adiabatic formalism has been derived, to study the DC, as well as the AC current, induced across an interacting quantum wire, regarded as a one-dimensional Luttinger liquid with pertinent parameters, connected to two superconductors at finite voltage bias  $V$ . In the equilibrium case, it has been shown that the main contribution to the equilibrium Josephson current comes from Andreev bound states at the Fermi energy, as a result of a nontrivial cancelation of the various contributions (these results are contained in a paper that will be soon submitted for publication). At variance, within the adiabatic formalism it has been possible to compute the current for any value of the tunneling amplitude between the contacts and the leads. In particular, using the Luttinger liquid description of interacting one-dimensional electronic systems, allowed for computing the current by also taking into account the interaction at the central region. Resorting to the boundary field theory formalism, then, allows for describing the effects of electron interaction onto the subgap current, due to multiple Andreev reflection processes.

## **9.5 INTEGRABILITY IN THE N=4 SUPERSYMMETRIC YANG-MILLS THEORY (SYM)**

In collaboration with D. Fioravanti, a first project was completed concerning twist operators in the  $sl(2)$  sector of planar  $N=4$  SYM in a special limit in which the relevant dynamics should be given by integral equations of the  $O(6)$  non-linear sigma model. Going into details, we compute anomalous dimensions by means of a nonlinear integral equation which is equivalent to the asymptotic Bethe Ansatz equations. We expand in powers of  $\ln S$ , where  $S$  is the semiclassical spin parameter. At the leading order  $\ln S$  we can re-confirm the  $O(6)$  non-linear sigma model description by Alday and Maldacena. By computing the first finite size correction  $1/\ln S$ , we find agreement with available string theory results at one loop and we give predictions for the two loops result.

A second project, in collaboration with D. Fioravanti and G. Infusino, concerns the study of reciprocity and functional relations in anomalous dimensions of twist operators in  $N=4$  SYM. We have verified that integrability agrees with reciprocity. These results are contained in the PhD Thesis of G. Infusino, defended in December 2011 and will be sent to the archives very soon.

## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2011**

1. M.S. Cardaci, P. Cea, L. Cosmai, R. Falcone and A. Papa,  
*Chromoelectric flux tubes in QCD*,  
Phys. Rev. D 83 (2011) 014502 [arXiv:1011.5803].
2. O. Borisenko, G. Cortese, R. Fiore, M. Gravina and A. Papa,  
*Numerical study of the phase transitions in the two-dimensional Z(5) vector model*,  
Phys. Rev. E 83 (2011) 041120 [arXiv:1011.5806].
3. A. Cirillo, M. Mancini, D. Giuliano, P. Sodano,  
*Enhanced Coherence of a Quantum Doublet Coupled to Tomonaga-Luttinger Liquid Leads*,  
Nucl. Phys. B 852 (2011) 235-268

#### **A.1.2 Publications on international journals accepted in 2011**

1. V.S. Fadin, R. Fiore, A.V. Grabovsky and A. Papa,  
*Connection between complete and Moebius forms of gauge invariant operators*,  
to appear on Nucl. Phys. B (2012) [arXiv:1109.6634 [hep-th]].

## **B PUBLICATIONS ON CONFERENCE PROCEEDINGS**

### **B.1 Publications on international conference proceedings in 2011**

1. A. Prokudin, R. Fiore, L.L. Jenkovszky, V.K. Magas, S. Melis,  
*Exclusive J/psi photo- and electroproduction in a dual model*,  
PoS DIS2010 (2010) 171; arXiv:1011.5924 [hep-ph].
2. N.G. Stefanis, I.O. Cherednikov, A.I. Karanikas,  
Role and properties of Wilson lines in transverse-momentum-dependent parton distribution functions,  
PoS (LC2010) 053; arXiv:1010.1934 [hep-ph].
3. P. Cea, L. Cosmai, M. D'Elia and A. Papa,  
*The critical line of QCD with four degenerate quarks*,  
PoS(Lattice 2010)173/1-7, arXiv:1012.4908 [hep-lat].
4. O. Borisenko, R. Fiore, M. Gravina and A. Papa,  
Critical behavior of the compact 3D U(1) gauge theory at finite temperature,  
PoS(Lattice 2010)188/1-7, arXiv:1012.4942 [hep-lat].
5. O. Borisenko, G. Cortese, R. Fiore, M. Gravina and A. Papa,  
Critical properties of the two-dimensional Z(5) vector model,  
PoS(Lattice 2010)274/1-7, arXiv:1101.0512 [hep-lat].

## **C PRESENTATIONS AT SCHOOL AND CONFERENCES**

### **C.1 Presentations at international schools and conferences in 2010**

1. I. Cherednikov,  
*What we need to evolve TMD correctly? Recent progress*,  
invited talk given at the "Gluons and the quark sea at high energies: distributions, polarization, tomography",  
Seattle (WA), USA, 13 Sept - 19 Nov 2010
2. I. Cherednikov,  
*Developments on unintegrated PDFs*,  
invited talk given at the 40th International Symposium on Multiparticle Dynamics,  
Antwerp (Belgium), 21 - 25 Sep 2010
3. I. Cherednikov,  
*Transverse momentum parton distributions: recent progress in theory*,

talk given at "Diffraction 2010", Otranto (Lecce), Italy, 10 - 15 Sep 2010

4. I. Cherednikov,  
*TMD parton densities: light-cone gauge calculations*,  
invited talk given at the International Workshop "Hadron Structure and QCD: from low to high energies",  
Gatchina, St. Petersburg, Russia, 5 - 9 Jul 2010
5. I. Cherednikov,  
*TMD factorization in light-cone gauges*,  
invited talk given at the International Workshop on Transverse Momentum Distributions (TMD 2010),  
Trento, Italy, 21 - 25 Jun 2010
6. I. Cherednikov,  
*Transverse-momentum dependent parton densities: definition, renormalization and evolution*,  
talk given at the 4th Workshop on Exclusive Reactions at High Momentum Transfer,  
Thomas Jefferson National Accelerator Facility Newport News (VA), USA, 18 - 21 May 2010
7. O. Borisenko, R. Fiore, M. Gravina and A. Papa,  
*Critical behavior of the compact 3D U(1) gauge theory at finite temperature*,  
poster presented by R. Fiore at LATTICE 2010, XVIII International Symposium on Lattice Gauge Theories,  
Villasimius, June 14 - 19, 2010.
8. O. Borisenko, G. Cortese, R. Fiore, M. Gravina and A. Papa,  
*Critical properties of the two-dimensional Z(5) vector model*,  
poster presented by G. Cortese at LATTICE 2010, XVIII International Symposium on Lattice Gauge Theories,  
Villasimius, June 14 - 19, 2010.
9. D. Giuliano,  
*Local pairing of Cooper Pairs in Josephson junction networks*,  
Plenary talk given at the ESF Research Conferences "Quantum Engineering of States and Devices: Theory and  
Experiments",  
Oberurg (Austria), 5-10 June 2010.
10. M. Rossi,  
*Integrability in N=4 SYM: the non linear integral equation approach*,  
poster presented at the international workshop RAQIS 2010, Annecy-le-Vieux (France), 15-18 June 2010.
11. M. Rossi,  
*Beyond cusp anomalous dimension from integrability in SYM4*,  
talk given at "Diffraction 2010", Otranto (Lecce), Italy, 10 - 15 Sep 2010.

#### **EDITORSHIP OF BOOKS**

1. M. Capua, R. Fiore, I. Ivanov, A. Papa, J. Soffer and E. Tassi,  
*Diffraction in high energy physics*,  
Proceedings of the International Workshop *Diffraction 2010*, Otranto, Italy, September 10-15, 2010,  
AIP Conf. Proc. 1350 (2011) 351 p.