



Dipartimento di FISICA



# **ANNUAL REPORT 2012**

ACADEMIC YEAR 2011 -2012 Scientific publications in 2012

> Università degli Studi della Calabria Dipartimento di Fisica C.da Arcavacata, Ponte P. Bucci - Cubo 31C 87036 RENDE (Cosenza) - ITALIA

# ANNUAL REPORT 2012

# ACADEMIC YEAR 2011-2012

Scientific publications in 2012

#### Quarant'anni nel dipartimento di Fisica dell'Università della Calabria

La presentazione del rapporto di attività del dipartimento di Fisica relativa all'anno 2012 è l'ultima della quale mi assumo la responsabilità nella veste di direttore del dipartimento. Dal 1 gennaio 2013, infatti, dopo nove anni di direzione ho passato il testimone al nuovo direttore prof. Riccardo Barberi.

Ho una particolare emozione nel redigere questa presentazione, perché nel dipartimento di Fisica ho trascorso quasi quarant'anni dall'ormai lontano 1974, quando a 25 anni, appena concluso il percorso di perfezionamento presso la Scuola Normale Superiore (all'epoca unica possibilità di conseguire un PhD in Italia), percorso che mi aveva anche portato a lavorare per due anni nell'*Osservatorio de Paris-Meudon*, ho preso servizio presso il dipartimento di Fisica come assistente ordinario.

Sono stati quarant'anni difficili e impegnativi sopratutto all'inizio: era necessario costruire praticamente dal nulla una nuova struttura di ricerca, didattica ed amministrativa, in una situazione molto particolare: i primi dieci anni di vita del dipartimento sono, infatti, stati caratterizzati dall'assenza di professori che avessero alle spalle una sufficiente esperienza, sicché un piccolo gruppo di giovanisimi ricercatori (Roberto Bartolino, Massimo Conti, Luigi Sportelli, Giovanni Falcone, Antonino Oliva, Cesare Umeton, Luigi Papagno oltre a me stesso), poco più che neolaureati, si è trovata sulle spalle responsabilità cui nessuno di loro era probabilmente preparato. Solo nel 1985 al gruppo iniziale si sono aggiunti alcuni professori ordinari vincitori di concorso, uno dei quali, il prof. Susinno, ha segnato in maniera estremamente significativa la vita del dipartimento, facendo nascere e svilupparsi all'interno del dipartimento stesso le attività di ricerca in Fisica della Alte Energie.

La redazione del Rapporto annuale di ricerca, che ormai da quasi trenta anni il Dipartimento di Fisica dell'Università della Calabria, prepara e distribuisce, fornisce una misura quantitativa di quanta strada il Dipartimento di Fisica abbia fatto in questi 40 anni. La sua prima edizione risale all'anno accademico 1986/87 ed era stata prodotta con una stampante ad aghi e successivamente fotocopiata e spillata nella segreteria del dipartimento. Da qualche anno il rapporto di attività, nella parte scientifica, è stato redatto in inglese, per facilitarne la diffusione anche tra i centri di ricerca internazionali.

Riguardando i rapporti anno per anno è possibile farsi un'idea di quanto e come il dipartimento di fisica sia cambiato in questo periodo. A parte alcune fluttuazioni c'è un chiaro trend di crescita, del dipartimento sia in termini di personale che di pubblicazioni: il personale di ruolo è passato dalle 25 unità del 1987 alle 46 unità del 2004, alle oltre 50 unità del 2012, ma accanto al personale di ruolo sono progressivamente comparsi, prima un consistente numero di dottorandi (dalle poche unità del 1997, fino alle oltre 30 unità dal 2004 in poi) poi un altrettanto consistente numero di assegnisti e borsisti post-doc (dalle poche unità degli anni tra il 1990 ed il 1999, fino alle circa 20 unità dal 2004 in poi). Il numero di pubblicazioni per anno su riviste internazionali, dedotte dai precedenti rapporti di attività, non ha cessato di crescere dalle poche decine degli anni '80, fino ad oltre 100 negli ultimi anni, mostrando che la crescita del dipartimento in termini di personale è stata accompagnata da una crescita ancora più accentuata in termini di produttività scientifica. Oggi il dipartimento di fisica rappresenta una consistente realtà nel panorama della ricerca nazionale ed internazionale, con settori che, anche dal punto di vista della massa critica di ricercatori, hanno ormai raggiunto una notevole visibilità.

La qualità della ricerca svolta all'interno del dipartimento ha avuto particolari e significativi riconoscimenti negli ultimi 2 anni, anzitutto attraverso i risultati della VQR 2004-2010. Mi piace ricordare qui alcuni dati: nella VQR il dipartimento di Fisica dell'Università della Calabria, limitato alla sola Area Fisica, ha riportato un punteggio medio di 0,89, che lo ha classificato al 3º posto tra i 30 dipartimenti di Fisica più grandi ed al 15º posto assoluto sui 78 dipartimenti italiani in cui l'Area Fisica è presente in entrambe le graduatorie nel primo quartile, risultato di tutto rispetto tenendo conto della eccellente collocazione internazionale della Fisica italiana; il dipartimento di Fisica post L240 è poi stato valutato in 3 SSD in cui sono presenti più di 4 tra professori e ricercatori (FIS/01, FIS/03, FIS/07) e in 2 di questi (FIS/03 e FIS/07) si è piazzato al primo posto in Italia. Primo posto assoluto con il punteggio di 0,96 per FIS/07, ex aequo con alcune tra le università italiane tradizionalmente più prestigiose (SISSA di Trieste e Milano-Politecnico) con il punteggio di 1 per FIS/03. Infine il recentissimo indice definito dalla commissione CRUI nazionale (Voto standardizzato) pone l'intero dipartimento di Fisica post L240 in testa ai dipartimenti dell'Università della Calabria assegnandogli un voto di 1,97 che misura, in termini di deviazioni standard, la posizione del dipartimento rispetto al valore medio nazionale di un dipartimento equivalente.

Anche i risultati dell'*Abilitazione Scientifica Nazionale* hanno fornito riscontri estremamente positivi sulla qualità dell'attività di ricerca svolta all'interno del Dipartimento di Fisica: 5 professori ordinari sui 9 del dipartimento hanno superato le soglie necessarie per far parte delle commissioni di abilitazione, 55,5% a fronte

di dati medi nazionali dell'ordine del 40%; 6 professori associati sui 18 (il 33,3%) afferenti al dipartimento hanno conseguito l'idoneità a professore ordinario; 11 ricercatori su 22 (il 50%) hanno conseguito l'idoneità a professore associato, idoneità che peraltro è stata conseguita anche da 4 dei nostri assegnisti.

Ulteriori segnali positivi: sull'ultimo FFO il MIUR ha espresso valutazione positiva alla chiamata diretta ed ha cofinanziato per l'Università della Calabria: 1 posto di professore ordinario (Sandra Savaglio sul settore FIS/05) ed 1 posto di professore associato (Giuseppe Strangi sul settore FIS/07) entrambi afferenti al dipartimento di Fisica; sull'ultimo bando PRIN, dotato di fondi ministeriali estremamente ridotti, solo 2 progetti con coordinatori nazionali dell'Università della Calabria (Vincenzo Carbone e Antonio De Luca) sono stati finanziati, anche in questo caso entrambi i coordinatori afferiscono al dipartimento di Fisica.

Torna infine conto segnalare che sui 15 professori dell'Unical presenti nella *Virtual Italian Academy* 9 sono o sono stati afferenti al dipartimento di Fisica.

Un discorso particolare merita poi il dottorato di ricerca in Fisica: coloro che hanno attivamente contribuito alla partenza del dipartimento di Fisica erano convinti che l'attivazione di un dottorato di ricerca rappresentasse l'unico strumento possibile per garantire la formazione di nuovi ricercatori e, attraverso lo scambio di dottorandi con istituzioni estere, l'internazionalizzazione della ricerca. Il dottorato in Fisica è stato attivato e finanziato dal Ministero della Ricerca Scientifica insieme a 2 soli altri dottorati dell'Unical fin dalla prima istituzione dei dottorati in Italia conseguente alla emanazione del D.P.R. 11 luglio 1980, n. 382, dapprima in Consorzio con l'Università di Messina e dopo pochi cicli in totale autonomia con il nome di "Dottorato di Ricerca in Fisica della Materia". A partire dall' VIII Ciclo (a.a. 1992/93) il dottorato si è poi allargato a "Dottorato di ricerca in Fisica". Dal 2005 le attività del dottorato sono confluite in parte nella Scuola "B. Telesio" ed in parte nella Scuola "Archimede" entrambe con sede amministrativa nel dipartimento di Fisica è stato attivato, in convenzione con il C.N.R. e con il contributo di alcuni gruppi di ricerca dell'Unical esterni al dipartimento (essenzialmente chimici ed ingegneri), un nuovo dottorato, che sulla base delle simulazioni realizzate dovrebbe essere in condizione di superare tutte le soglie di qualità, in corso di definizione da parte dell'ANVUR, per l'accreditamento dei dottorati italiani.

Gli anni che ci si prospettano debbono essere quelli del consolidamento dei risultati raggiunti. Questo obiettivo richiederà lo sforzo concorde e convinto di tutto il personale del dipartimento, in particolare, a mio parere, il dipartimento dovrà impegnarsi nella ristrutturazione dell'offerta didattica proponendo ai potenziali studenti, accanto ad un solido Corso di laurea in Fisica, un Corso triennale destinato a formare laureati esperti nell'utilizzo delle nuove tecnologie fisiche e/o nelle applicazioni della Fisica a quelle attività economiche che già sono presenti nel territorio calabrese.

Arcavacata di Rende, 31 gennaio 2014

Pierluigi VELTRI

# **Table of Contents**

# **GENERAL INFORMATION**

Departmental Administration	7
Research Permanent Staff	8
Post-Doctoral Research Fellows, Phd Students	8
Technical And Administrative Staff	10
Department Phonebook	11
Seminars	12
Laurea Thesis'	14
1 st level degree thesis'	14
2nd level degree thesis'	16
Phd thesis'	18

# RESEARCH ACTIVITY

<b>1</b> 1.1	ASTROPHYSICS MAGNETOHYDRODYNAMIC TURBULENCE AND KINETIC EFFECTS IN	19
	THE INTERPLANETARY SPACE	. 21
1.2	OBSERVATIONS AND TURBULENCE MODELS IN THE SOLAR ATMOSPHERE	26
1.3	MAGNETOSPHERIC PHENOMENA AND GEOPHYSICS	28
1.4	LABORATORY PLASMAS	29
	Publications	31
2	BIOMEDICAL PHYSICS	37
2.1	DOSIMETRY WITH NOVEL EPR-SENSITIVE MATERIALS	36
2.2	STUDY OF RADIATION EFFECTS IN BIOMOLECULE OF DOSIMETRIC INTEREST	38
	Pubblications	33
3	CONDENSED MATTER PHYSICS	41
3.1.	SURFACE NANOSCIENCE	42
3.2	ION INDUCED AND ELECTRON INDUCED EXCITATIONS IN	
	GRAPHENE/SUBSTRATE SYSTEM SAND CARBON NANOTUBES	44
3.2.1	Collective response of low dimensional, many body systems to an abrupt perturbation	44
3.2.2	Electronic properties and plasmon excitations in Graphene and doped grapheme	44
3.2.3	Abinitio simulations and spectroscopy of Graphene/Metal interfaces	44
3.2.4	ARSEE Experiments on Graphene	45
3.3	PHOTON-MATTER INTERACTION: ELECTRONIC PROPERTIES OF GRAPHENE	
	AND RELATED MATERIAL	45
3.4	QUANTUM COHERENCE AND CORRELATIONS IN CONDENSED MATTER	
	SYSTEMS	46
3.5	ION-MATTER INTERACTION	46
3.5.1	Ion interaction with nanostructures.	46
3.5.2	Radiation interaction with solids	47
3.5.3	Diagnostic in cultural heritage	47
3.5.4	New materials growth for application to Graetzel photoelecrochemical cells	48
3.6	PHYSICS EDUCATION RESEARCH (PER)	48
	Publications	50
4	EXPERIMENTAL PARTICLE PHYSICS	55
4.1	THE ZEUS EXPERIMENT AT HERA E-P COLLIDER (DESY, HAMBURG-GERMANY)	55
4.2	ATLAS EXPERIMENT AT THE LHC P-P COLLIDER (GENEVA-SWITZERLAND)	56
4.3	HADRONIC CALORIMETRY	59
4.4	3D PIXEL COLLABORATION	61
4.5	KLOE-2 EXPERIMENT AT DAFNE E-E+ COLLIDER (National Laboratory of Frascati)	61
4.6	AIR SHOWER OBSERVATORY WITH SCINTILLATOR DETECTORS ARRAY	61
	Publications	63

5	MOLECULAR BIOPHYSICS	77
5.1	TRANSPORT PROTEINS/LIGANDS COMPLEXES	77
5.1.1	Interaction of resveratrol with transport proteins	77
5.1.2	Molecular dynamics and docking of fatty acids interacting with beta-lactoglobulin	78
5.2	AGGREGATION AND GLASSY BEHAVIOUR OF MODEL PROTEINS	79
5.2.1	Effects of the presence of metal ions on the aggregation of beta-lactoglobulin	79
5.2.2	Glassy behavior of proteins	79
5.3	MOLECULAR INTERACTION AT THE LIPID/PROTEIN INTERFACE	80
5.3.1	Association of alpha-synuclein and mutants with lipid membranes	80
5.3.2	Water penetration profile at the protein-lipid interface in Na,K-AI Pase membranes	80
5.3.3	Protein marker in food biotechnology	81
(	Publications	82 04
0	MATERIALS IN CLOSE COLLARODATION WITH CHEMIST CROUPS, DOTH	84
0.1	MATERIALS, IN CLUSE CULLABORATION WITH CHEMIST GROUPS, BUTH	
	COLLOIDAL SYSTEMS, NANODADTICLES AND LIQUID CRYSTALS,	
	POLVMERS PHOTOPOLVMERS BLENDING OF LIQUID CRYSTALS,	
	POLYMERS, THOTOLOLIMERS, BLENDING OF EIQUID CRISIALS AND POLYMERS CHARACTERISATION (DIELECTRIC RAMAN ELLIPSOMETRY	
	FI FCTRON MICROSCOPY )	86
611	Application of Raman spectroscopy to the characterization of solids, thin films, soft matter	80
0.1.1	as well as artifacts of cultural heritage	87
612	Non Debye relevation in the dielectric response of nematic liquid crystals: Surface and memory	07
0.1.2	Non-Debye relaxation in the dielectric response of nematic riquid crystals. Surface and memory	00
	effects in the adsorption-desorption process of ionic impurities	88
6.1.3	Fractional Diffusion Equation and the Electrical Impedance: Experimental Evidence in	
	Liquid-Crystalline Cells.	88
6.1.4	Dielectric investigations on new bent-core liquid crystal	89
6.1.5	Dielectric Characterisation of an Orthoconic Antiferroelectric Liquid Crystal Mixture	89
6.1.6	Flexoelectro-Optical Behaviour of Layers Formed by Polymer-Liquid Crystal Phase-Separated	
	Composites	90
6.1.7	Tailoring the physical properties of polymeric nanocomposite films by the insertion of graphene and metal nanoparticles	. 90
6.1.8	Ferroelectric switching in the cybotactic nematic phase of a main-chain liquid crystal polymer with	
	hent-core monomeric unit	91
610	Chaning supromalocular shirality in smort nalymore with 2D Dalarization Light Detterns	02
0.1.9	Shaping supramolecular chirality in small polymers with 2D Polarization Light Patients	93
6.1.10	Programmable microlens arrays by single-step polarization holographic recording in photosensitive	
	soft materials	94
6.1.11	Chiral Self-assembled solid microparticles	94
6.2	SURFACES AND INTERFACES: CHARACTERISATION, INTERACTION LC-SURFACES,	
	POLYMER SURFACES, ANCHORING, EFFECTS ON ELECTROOPTICS AND PHOTONICS	94
6.2.1	Investigation and Applications of POLICRYPS Gratings	94
6.2.2	A Novel Polymer Matrix for Confinement and Alignment of Self-Organized Materials	95
6.2.3	Realization and characterization of photonic aperiodic structures with a photo-polymerization	
	Technique	95
6.2.4	POLICRYPS Gratings with metallic nano-inclusions towards Metamaterials	95
6.2.5	Active Plasmonic systems realized in soft elastomers coated with gold NPs layers	96
6.2.6	Electro-switchable soft materials for photonic applications	97
6.2.9	Dielectric Spectroscopy of Soft Matter	97
6.3	CONFINED SYSTEMS, NANOSCIENCES, PHOTONICS: LASING, GRATING,	
	MEMORIES, HOLOGRAPHY, POLYCRIPS, SOLITONS	7
6.3.1	Loss Compensation Routers in Matamaterials Sub-Units	97
6.3.2	Polymer based Diffraction gratings.	98
6.3.3	Study of microparticles with anisotropic optical properties and also chiral, that combines	0.5
	The science of soft matter photonics and optical manipulation 1	00
6.3.4	Lasing in photonic bandgap materials based on liquid crystals doped with fluorescent dyes	0.1
<pre></pre>	In liquid crystalline phases (Cholesteric blue-phase) 1	01
6.3.5	Generation of complex beams by means of polarization holograms	101
0.3.6	Liquid Crystal Based Polarization Gratings for Spectro-polarimatric Applications	101

6.4	NANO-IMAGING OF BIOLOGICAL AND BIOCOMPATIBLE MATERIALS AND	
	SURFACE FORCE APPARATUS (SFA)	101
6.4.1	Periodic Defect Patterns And Guided Nanoparticle Assembly In Smectic Liquid Crystal Films	101
6.4.2	Nanoscience and biomedicine	102
6.4.3	Nanomechanics and nanotribology of adhesive and lubricating protein layers	103
	Publications	104
7	SURFACE ELECTRON SPECTROSCOPY (SPES)	109
7.1	GRAPHENE/METAL INTERFACES	110
7.1.1	Vibrati Dispersion and Damping Processes of $\pi$ Plasmon in Monolayer Graphene	110
7.1.2	Evidence of Kohn anomalies in quasi-freestanding graphene on Pt(111)	110
7.1.3	Phonon dispersion of quasi-freestanding graphene on Pt(111)	111
7.1.4	Effects of a humid environment on the sheet plasmon resonance in epitaxial grapheme	111
7.1.5	Elastic properties of a macroscopic graphene sample from phonon dispersion measurements	111
7.2	SPECTROSCOPIC AND MICROSCOPIC STUDIES OF CARBON AND METAL-OXIDE	
	NANOSTRUCURES	111
7.2.1	ZnTPP dye adsorption on nanostructured TiO <sub>2</sub>	111
	Publications	113
8	THEORETICAL PARTICLE PHYSICS AND APPLICATIONS	114
8.1	QCD IN THE HIGH-ENERGY LIMIT AND HADRON PHENOMENOLOGY	115
8.1.1	QCD in the high-energy limit	115
8.1.2	Hadron Phenomenology	115
8.2	LATTICE GAUGE THEORIES	116
8.2.1	Finite density QCD	116
8.2.2	Confinement in QCD	116
8.2.3	Berezinsky-Kosterlitz-Thouless (BKT) phase transitions in spin models	116
8.2.4	Planar QED in external fields	117
8.3	FIELD THEORY OF CORRELATED DEVICES	117
8.3.1	Junctions of interacting quantum wires and mathematical model for SNS junctions made with topological superconductors	117
8.3.2	Spin-chain representation of the lattice Bose-Hubbard chain	117
8.3.3	Topogical Kondo effect due to emerging Majorana modes in Josephson junction networks	118
	Topogreat Rondo effect due to emerging Majorana modes in soseptison junction networks	110
8.4	INTEGRABILITY IN THE <i>N</i> =4 SUPERSYMMETRIC YANG-MILLS THEORY (SYM)	118

#### 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:**

- 9 Full Professors
- 18 Associate Professors
- 23 Senior Researchers
- 24 Representatives of Post-Doctoral Research Fellows
- 10 Representatives of PhD students
- 5 Representatives of the Technical and Administrative Staff

# Administrative Secretary:

Gaspare PECORA

#### **RESEARCH PERMANENT STAFF**

Full Professors	
1. Riccardo BARBERI	<i>FIS/07</i>
2. Roberto BARTOLINO	<i>FIS/07</i>
3. Vincenzo CARBONE	<i>FIS/07</i>
4. Elio COLAVITA	<i>FIS/07</i>
5. Giovanni FALCONE	<i>FIS/01</i>
6 Ignazio GUERRA	GEO/10
7 Luigi SPORTELLI	FIS/07
8 Cesare LIMETON	FIS/01
9 Pierluigi VELTRI	FIS/03
7. Thermale VELTIC	115/05
Associata Professors	
1 Poffoele ACOSTINO	
2 Desine DADTUCCI	FIS/01 EIS/07
2. Rosina DARI UCCI	FIS/07
4. Loronzo CADUTI	F15/01 F15/01
4. LOICHZO CAPUTI	F15/01
5. Enzo CAZZANELLI	F15/05
6. Gennaro CHIARELLO	F1S/07
/. Gabriella CIPPARRONE	F15/03
8. Giovanni CROSETTI	F1S/01
9. Laura LA ROTONDA	F1S/01
10. Francesco MALARA	FIS/01
11. Alessandro PAPA	FIS/02
12. Francesco PIPERNO	FIS/03
13. Nicola SCARAMUZZA	FIS/07
14. Marco SCHIOPPA	<i>FIS/01</i>
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/01
11 Antonella GRECO	FIS/02 FIS/07
12 Dite CUZZI	FIS/07
12. KILA OUZZI 12. Endria I EDDETI	F15/07 F15/02
13. FAULO LEFKEII	F15/05 F15/01
14. Anna MASIOBERARDINO	F15/01
15. Daniela PACILE	F1S/01
16. Pasquale PAGLIUSI	FIS/0/
17. Marco PAPAGNO	ELG (A 1
18. Francesco PLASTINA	FIS/01
19. Leonardo PRIMAVERA	FIS/05
20. Pierfrancesco RICCARDI	FIS/01
21. Marco ROSSI	FIS/02
22. Antonello SINDONA	FIS/01
23. Giuseppe STRANGI	<i>FIS/07</i>
24. Francesco VALENTINI	FIS/03

#### **Post-Doctoral Research Fellows**

- Tony John George APOLLARO 1.
- Manuela BRUNO Marco CASTRIOTA
- 2. 3.
- 4. Serena DALENA
- 5. Francesco FRANCICA
- 6. Ridha HAMDI
- 7. Melissa INFUSINO
- 8. Hari Krishna KODURU
- 9. Lorenzo SALVATORE
- 10. Giuseppina NIGRO
- 11. Manuela PANTUSA
- 12. Silvia PERRI

- Gia PETRIASHVILI
  Luigia PEZZI
  Valentino PINGITORE
- 16. Antonio POLITANO
- Antonio POLITANO
  Clementina PROVENZANO
  Giuseppe PUCCI
  Ulises RUIZ CORONA
  Daniela SALVATORE
  Sergio SERVIDIO
  Sergio SERVIDIO

- 22. Antonio VECCHIO
- Alessandro VELTRI
  Tommaso VENTURELLI

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

(XXV Cycle)
(XXV Cycle)
(XXV Cycle)
(XXV Cycle)
(XXVI Cycle)
(XXVI Cycle)
(XXVI Cycle)
(XXVI Cycle)
(XXVI Cycle)
(XXVII Cicle)
(XXVII Cicle)
(XXVII Cicle)
(XXVII Cicle)

# Phd School "Science and Thecnique": Curriculum

"Physics of Complex Systems"	-
1. Vincenzo CAPPARELLI	(XXV Cycle)
2. Denise PERRONE	(XXV Cycle)
3. Enrico Maria TROTTA	(XXV Cycle)
4. Loris D'ALESSI	(XXVI Čycle)
5. Gaetano DE VITA	(XXVI Cycle)
6. Christian Natale GENCAREL	LI (XXVI Cycle)
7. Stefania EVOLI	(XXVII Cicle
8. Luca TIRIOLO	(XXVII Cicle

#### Phd School "Science and Thecnique": Curriculum "Science and Tecnologies of Mesophases and Molecular Materials'

1. Angela FASANELLA	(XXV Cycle)
2. Raul Josuè HERNANDEZ	(XXV Cycle)
3. Lucia MARINO	(XXV Cycle)
4. Teresita de Jesus CALDERA	LOPEZ (XXVI Cycle)
5. Manuela CATALANO	(XXVI Cycle)
6. Ugo CATALDI	(XXVI Cycle)
7. Eugenia LE PERA	(XXVI Cycle)
-	

(XXVI Cycle)
(XXVI Čycle)
(XXVI Cycle)
(XXVI Cycle)
(XXVII Cycle)
(XXVII Cycle)
(XXVII Cycle)
(XXVII 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 INFM Section with the following staff: Sonia VIVONA (*Administrative Official - INFM*) Antonio BOZZARELLO (*Administrative Collaborator*)

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

# INTERNET: @FIS.UNICAL.IT HTTP: WWW.FIS.UNICAL.IT FAX: 4401

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

#### SEMINARS (2012)

Jen 10, 2012 Dr.ssa Lucia Votano, Laboratori Nazionali Gran Sasso - INFN La fisica del neutrino al Laboratorio sotterraneo del Gran Sasso

Feb 2, 2012 Prof. Luca Caneschi, INFN-Ferrara Anomalie chirali

*Feb 8, 2012* Dr. Giulio Caracciolo, Dipartimento di Medicina MolecolareUniversità di Roma "La Sapienza" *Lipid-mediated gene transfer: state-of-the-art and perspectives* 

Mar 7, 2012 Dr. Gabriele Campagnano Formalismo di Landauer, conduttanza vista come scattering

Mar 7, 2012 Dr. Gabriele Campagnano Applicazioni del formalismo di Landauer; Formalismo di Keldysh di non equilibrio

May 25, 2012 Prof. Wieslaw Macek, University, Varsavia Observation of the multifractal spectrum at the termination shock by Voyager 1- parte prima

May 28, 2012 Le ricerche dello SM Higgs ad ATLAS Dr. Evelin Meoni (Tufts University)

May 29, 2012 Prof. Wieslaw Macek, University, Varsavia Observation of the multifractal spectrum at the termination shock by Voyager 1 - parte seconda

Jun 6, 2012 Prof. I.C. Khoo, PennState University Active plasmonics based metamaterials

*Jul 6, 2012* Dr. Carlos Peña Garay, Instituto de Fisica Corpuscular – Valencia *Neutrino Flavor Conversion,* 

Sep 28, 2012 Prof. Rainer Schicker, Univ. Heidelberg Central diffraction - From the ISR to the LHC

*Oct 9, 2012* Prof. Igor Ivanov, Universite' de Liege, and Sobolev Institute of Mathematics (Novosibirsk) *Probing the phase of the scattering amplitude via vortex beams* 

Oct 17, 2012 Prof. Derek Marsh, Max Planck Institute for Biophysical Chemistry - Goettingen - Germany Lipid Rafts and Lipid-Protein Interactions in Membranes Oct 30,2012 Dr. J. Goold, Clarendon Laboratory, University of Oxford Emergent Thermodynamics in many-body systems

Nov 22, 2012 Dr. Christian Torrero, Universita` di Parma *A numerical study of the Bose-Hubbard model with a trapping potential* 

Dec 6, 2012 Dr. G.A. Chirilli (Ohio State University) Linear and Non-linear Dynamics of Quantum Chromodynamics at High-Energy

Dec 13, 2012 prof. Paternostro, Queen's University, Belfast Distribuzione di entanglement tramite stati separabili

Dec 17, 2011 Dr. Lajos Molnar, University of Debrecen (Hungary) Preserver problems on Quantum Structures

# LAUREA THESIS' in 2012

#### **1st LEVEL DEGREE THESIS' IN 2012**

#### Apr 24

Veronica SPADAFORA Analisi del tremore sismico nel comune di Cosenza Relatore: Gaetano ZIMBARDO

#### May 9

Marina D'AMICO Dosimetria con fascio elettronico per radioterapia. Relatore: Anna MASTROBERARDINO

#### Serena PERRI

La tecnica emanometrica per la misura di concentrazione di Radon in aria e acqua ed il suo contributo alla ricerca in ambito sanitario Relatore: Marcella CAPUA

Diego ALESSIO Applicazione del p-model al flare di raggi gamma registrato nella Nebulosa Granchio nel settembre 2011 RelatoreFabio LEPRETI

Francesca ALESSANDRO Nanomagneti accoppiati in un risonatore elettromagnetico Relatore: Francesco PLASTINA

Sara RESTUCCIA Numerical Simulations of Alpha-Omega Dynamos Relatore: Vincenzo CARBONE

Francesco NACCARATO Effetti non lineari in processi di fotoemissione in sistemi nanostrutturati a base di carbonio Relatore:Antonio SINDONA

Martina DE STEFANO Il principio variazionale in meccanica quantistica: teoria e applicazioni Relatore: Marco ROSSI

Donatello PAGNOTTO Misura della Concentrazione di Radon in Acque Sorgive Relatore: Marcella CAPUA

*May 11* Veronica GATTO *La viscosità degli oli lubrificanti per motore* Relatore: Cesare UMETON

Alessio DE MARCO Synthesis of Noble - and non Noble Metals on Carbon Black Catalyst Support for PEM Fuel Cell Relatore: Gennaro CHIARELLO

July 24 Gianluca GRECO Studi Monte Carlo sulla produzione di particelle esotiche a lunga vita media Relatore: Enrico TASSI Sep 24 Caterina PELLEGRINO La soluzione esatta della catena di Heisenberg Relatore: Marco ROSSI

Valeria PARISE Algoritmi cellulari neurali per la diagnostica medica Relatore: Anna MASTROBERARDINO

Federica GARZANTI *Propagazione ondosa in cromosfera e corona* Relatore: Francesco MALARA

Francesco COSCO Decoerenza quantistica in ambiente di bosoni condensat Relatore: Francesco PLASTINA

Giuseppe CALLEA *I Maxwelliani e la produzione di onde elettromagnetiche* Relatore: Enrico TASSI

Giulio RICHICHI Biosensori cellulari Relatore: Anna MASTROBERARDINO

Jessica CASTAGNA Misure di concentrazione di Rn-222 mediante celle di Lucas e fattori correttivi della statistica di conteggio Relatore: Marcella CAPUA

Sep 28 Sara DE CICCO Compensazione delle perdite ottiche in nanostrutture metalliche assistite da materiali di guadagno per la realizzazione di metamateriali Relatore: Giuseppe STRANGI

#### Oct 23

Giusi CUTULI Misure ambientali di Radon Relatore: Anna SANTANIELLO

#### Dec 13

Giuseppe MANDILE *Caratteristiche del suono e misure di randon per la valutazione del rischio* Relatore: Anna SANTANIELLO

Pietro RAGNO Tecniche di costruzione in relazione alla mappe del rischio Radon Relatore: Anna SANTANIELLO

#### Dec 19

Renzo PUCCI Studio dell'interazione dell'acqua con un singolo strato di grafene cresciuto su una superficie di Ru (0001 Relatore: Vincenzo FORMOSO

#### Dec 20

Antonio Giovanni BRUNO Il teorema di Wigner in meccanica quantistica Relatore: Giuseppe NISTICO' Eduardo D'IPPOLITO Determinazione delle costanti dielettriche di nematici puri ed in miscele Relatore: Carlo Consolato VERSACE

Vincenzo BRUNO Bio-nano organizzazione di nanoparticelle d'oro mediante DNA liquido cristallino Relatore: Luciano DE SIO

Emanuele REDA Esperimenti di spettroscopia elettronica su film sottili di NiO (100) Relatore: Pierfrancesco RICCARDI

Gaetana ANAMIATI Inclusione all'ordine dominante della ZO nel Monte Carlo DISENT Relatore: Alessandro PAPA

Federica CHIAPPETTA Dinamica del clima terrestre: relazioni Sole – Terra Relatore: Vincenzo CARBONE

Luigi RIZZO Conseguenze dell'equazione di Boltzmann per un sistema di eventi quantistico relativistico Relatore: Pieluigi VELTRI

Elena LONGO Sistemi biomimetici per "drug delivery" Relatore: Rosa BARTUCCI

Francesco VISCOMI Diffractive behaviour of a POLICRYPS infiltrated with Gold nano particles doped Cholesteric Liquid Crystals Relatore: Roberto CAPUTO

Jacopo SETTINO Una misura della non - Markovianità dell'Evoluzione Quantistica Relatore: Francesco PLASTINA

Domenico TROTTA Smorzamento non collisionale delle onde nei plasmi: soluzioni asintoniche e transienti Relatore: Francsco VALENTINI

Davide MICIELI Studio della corda vibrante non lineare Relatore: Enrico TASSI

Emanuele BEVACQUA Focus sull'ultima Glaciazione Relatore: Vincenzo CARBONE

#### **2st LEVEL DEGREE THESIS' IN 2012**

*Mar 28* Rosanna CARNEVALE *Interazione tra il vento solare e il campo magnetico terrestre: dinamica del plasma magnetosferico* Relatore: Gaetano ZIMBARDO May 8 Maria Chiara ANGIOCCHI Protocollo di misura e analisi dati di concentrazione di radon acqua Relatore: Marcella CAPUA

Antonio MANDARINO Correlazioni quantistiche in una catena XX in campo trasverso Relatore: Francesco PLASTINA

Francesco Demetrio MINUTO Oltre il monolayer. Sviluppo di un dispositivo per la caratterizzazione Raman di H2 condensato Relatore: Raffaele Giuseppe AGOSTINO

Domenico GIAMPA' *Comportamento del plasma nell'RFP* Relatore: Leonardo PRIMAVERA

Amino Adelmo LAVORINI Models the exclusive diffractive production of real photons and vector mesons in a factorized Regge-pole framework Relatore: Roberto FIORE

Carla ESPOSITO Analisi dei processi di adsorbimento in setacci molecolari SAPO-34 per la separazione CO2/CH4 in membrane ibride Relatore: Raffaele Giuseppe AGOSTINO

Alessandro CRISTALLO Transizione confinamento-deconfinamento in sistemi elettronici correlati Relatore: Domenico GIULIANO

Andrea GNISCI Adsorbimento di molecole coloranti su superfici nanostrutturate di ossido di titanio Relatore: Raffaele Giuseppe AGOSTINO

Jul 17

Antonio FERRARO Realization and characterization of nanostructured luminescent materials Relatore: Roberto CAPUTO

Antonio POLITANO Studio delle proprieta' elettroniche, vibrazionali e della reattivita' chimica di grafene su superfici metalliche Relatore: Gennaro CHIARELLO

#### *Oct 2*

Ersilia LEONARDIS Universal characteristics og MHD turbulence in the poler solar wind as seen by Ulysses Relatore: Vincenzo CARBONE

Victor LAZZAROLI Assorbimento e trasmissione di nanoparticelle metalliche accoppiate ad un materiale di guadagno Relatore: Francesco PLASTINA

Andrea NAVA Boundary Phase Diagram of a Y - junction of Interacting Quantum WiresRelatore Relatore: Domenico GIULIANO

Francesco PUCCI Numerical Simulations of Magnetohydrodynamic Waves Relatore: Francesco MALARA **Dec 4** Francesco Giovanni CELIBERTO Inclusione all'ordine sottodominante della Z0 nel Monte Carlo DISENT Relatore: Alessandro PAPA

Francesca CUTERI Chromoelectric flux tubes in QCD Relatore: Alessandro PAPA

#### PhD THESIS' in 2012

(24° Ciclo) Silvia SALSONE *Bio-Optics, optical systems for diagnostics. Near-Infrared Imaging technique for detection of dental demineralisation* Supervisore: Giuseppe LOMBARDO

(25° Cycle) Enrico Maria TROTTA A levy walk approach to the propagation of solar energetics particles Supervisore: Zimbardo

(25° Cycle) Denise PERRONE A kinetic multi-component numerical model for the solar wind small-scale turbulence Supervisore: Pierluigi VELTRI

(25° Cycle) Vincenzo LAVORINI Study of the top quark differential cross section with the ATLAS detector at the LHC Supervisore: Prof. Enrico TASSI

(25° Cycle) Michele PISARRA Electronic Excitation of Graphene, Graphene Nickel interfaces, and Carbon Nanotubes Supervisori: Dr. Pierfrancesco RICCARDI e Dr. Antonello SINDONA

(25° Cycle) Beatrice MURDACA Forward jets at LHC in pQCD Supervisore: Prof. Alessandro PAPA

(25° Cycle) Lucia MARINO Dielectric Characterization of Different Mesogenic Substances and a Mixture with Non-conventional Gold Nanoparticles Supervisore:

(25° Cycle) Josuè Raul HERNANDEZ Optical Trapping and Manipulation Exploiting Optical Crystalline Systems Supervisore: Gabriella CIPPARRONE

(25° Cycle) Angela FASANELLA Micro Raman Spectroscopic Investigations on Soft Matter Systems Supervisore: Enzo CAZZANELLI

# 1. ASTROPHYSICS

Professors and	
Researchers	Pierluigi Veltri Vincenzo Carbone Francesco Malara Gaetano Zimbardo
	Leonardo Primavera
	Antonella Greco
	Fabio Lepreti Francesco Valentini
	Luca Sorriso-Valvo (LICRYL, IPCF-CNR Cosenza)
	Grigol Gogoberidze
Postdoc fellows	Antonio Vecchio
	Marco Onotri Sergio Servidio
	Giuseppina Nigro
	Silvia Perri
	Serena Dalena
PhD students	Denise Perrone
	Enrico Maria Trotta
	Loris D'Alessi
	Gaetano De Vita
	Francesco Pucci
Collaborators	P. Pommois (Dipartimento di Fisica, Università della Calabria, Rende, Italy)
	I. Guerra (Dipartimento di Fisica, Università della Calabria, Rende, Italy) E. Califano (Dipartimento di Fisica, Università di Pisa, Pisa, Italy)
	F. Pegoraro (Dipartimento di Fisica, Università di Pisa, Pisa, Italy)
	M. Velli (Dipartimento di Fisica e Astronomia, Università di Firenze, Italy)
	M. Romé (Dipartimento di Fisica and INFN, Università di Milano. Italy)
	R. Pozzoli (Dipartimento di Fisica and INFN, Università di Milano. Italy) G. Maero (Dipartimento di Fisica and INFN, Università di Milano, Italy)
	B. Paroli (Dipartimento di Fisica and INFN, Università di Milano. Italy)
	F. Cavaliere (Dipartimento di Fisica and INFN, Università di Milano. Italy)
	M. Ikram (Dipartimento di Fisica and INFN, Università di Milano. Italy)
	R. D'Amicis (IFSI - CNR, Frascati, Italy) R. D'Amicis (IFSI - CNR, Frascati, Italy)
	M. Laurenza (IFSI - CNR, Frascati, Italy)
	M. Storini (IFSI - CNR, Frascati, Italy)
	M. Cavenago (INFN Laboratori Nazionali di Legnaro, Italy) G. De Masi (Consorzio REX: Associazione EURATOM-ENEA sulla Eusione, Padova
	Italy)
	M. Anzidei (Istituto Nazionale di Geofisica e Vulcanologia, Roma, Italy)
	F. Sahraoui (Laboratoire de Physique des Plasmas, CNRS-Ecole Polytechnique-UPMC, Observatoire de Saint Maur Saint Maur des Fosses France)
	D. Meduri (Max-Planck-Institut für Sonnensystemforschung, Katlenburg-Lindau, Germany)
	G. Nisticò (Centre for Fusion, Space and Astrophysics, Warwick University, Coventry, UK)
	S. C. Chapman (Centre for Fusion, Space and Astrophysics, Warwick University, Coventry, UK)
	B. Filia (Centre for Fusion, Space and Astrophysics, Warwick University, Coventry, UK) M. W. Dunlop (Centre for Fusion, Space and Astrophysics, Warwick University, Coventry, UK)
	A. J. Turner (Centre for Fusion, Space and Astrophysics, Warwick University, Coventry, UK)
	L. M. Zelenyi (Space Research Institute, Russian Academy of Sciences, Moscow, Russia)

R. Kovrazhkin (Space Research Institute, Russian Academy of Sciences, Moscow, Russia) M. Dolgonosov (Space Research Institute, Moscow, Russia) G. Aburjania (Nodia Geophysics Institute, Tbilisi University, Georgia) O. Kharshiladze (Tbilisi State University, Georgia) W. H. Matthaeus (Bartol Research Institute, Newark, Delaware, USA) M. Shay (Bartol Research Institute, Newark, Delaware, USA) M. Wan (Bartol Research Institute, Newark, Delaware, USA) F. Rappazzo (Bartol Research Institute, University of Delaware, Newark, Delaware, USA) K. T. Osman (University of Delaware, Newark, USA) P. Cassak (Department of Physics, West Virginia University, USA) A. Pouquet (National Center for Atmospheric Research, Boulder, Colorado, USA) D.C. Montgomery (Department of Physics and Astronomy, Dartmouth College, Hanover, New Hampshire, USA) V. I. Abramenko (Big Bear Solar Observatory, USA) V. Yurchyshyn (Big Bear Solar Observatory, USA) P. R. Goode (Big Bear Solar Observatory, USA) T. M. O'Neil (Department of Physics, University of California at San Diego, USA) P. J. Morrison (Department of Physics and Institute for Fusion Studies, University of Texas, Austin, USA) M. L. Goldstein (NASA-Goddard Space Flight Center, Greenbelt, Maryland, USA) J. C. Dorelli (NASA-Goddard Space Flight Center, Greenbelt, Maryland, USA) H. Korth (The Johns Hopkins University Applied Physics Laboratory, Laurel, Maryland, USA) T.H. Zurbuchen (Department of Atmospheric, Oceanic, and Space Sciences, University of Michigan, Ann Arbor, Michigan, USA) R. L. Mace (School of Chemistry and Physics, University of KwaZulu-Natal, Westville Campus, South Africa) P. Dmitruk (Departemento de Fisica, Universitad de Buenos Aires, Argentina) D. Ruffolo (Department of Physics, Mahidol University, Bangkok, Thailand) P. Chuychai (School of Science, Mae Fah Luang University, Thailand) G. Qin (State Key Laboratory of Space Weather, Center for Space Science and Applied Research, Chinese Academy of Sciences, Beijing, China) S. Oughton (Department of Mathematics, University of Waikato, New Zealand)

#### 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; Firenze) and with Italian Institutions (IFSI - CNR of Frascati; INFN Laboratori Nazionali of Legnano, Italy; Consorzio RFX of Padova; Istituto Nazionale di Geofisica e Vulcanologia of Roma) and foreign Institutions (CNRS, Laboratoire de Physique des Plasmas, Saint-Maur-des-Fosses, France; Max-Planck-Institut für Sonnensystemforschung, Katlenburg-Lindau, Germany; Centre for Fusion, Space and Astrophysics, Warwick University, Coventry, UK; Space Research Institute, Moscow, Russia; Nodia Geophysics Institute and Tbilisi University, Georgia; Bartol Research Institute, Newark, Delaware, USA; University of Delaware, Newark, USA; Department of Physics, West Virginia University, USA; National Center for Atmospheric Research, Boulder, Colorado, USA; Dartmouth College, Hanover, New Hampshire, USA; Big Bear Solar Observatory, USA; Department of Physics, University of Texas, Austin, USA; NASA Goddard Space Flight Center, Greenbelt, MD, USA; The John Hopkins University Applied Physics Laboratory, Laurel, USA; Department of Atmospheric, Oceanic, and Space Sciences, University of Michigan, Ann Arbor, USA; Departmento de Fisica, Universitad de Buenos Aires, Argentina; School of Chemistry and Physics, University of

KwaZulu-Natal, Westville Campus, South Africa; Department of Physics, Mahidol University, Bangkok, Thailand; School of Science, Mae Fah Luang University, Thailand; Center for Space Science and Applied Research, Chinese Academy of Science, Beijing, China; Department of Mathematics, University of Waikato, New Zealand).

The specific research themes under study during the year 2012 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 and Hall 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 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.

#### Detection of magnetic discontinuities in the high-frequency range of solar wind turbulence.

Thanks to recent high resolution spacecraft observations it has been possible to detect the existence of a cascade of magnetic energy in the solar wind plasma from the scale of the proton Larmor radius down to the one of the electron Larmor radius. However, the shape and the decay rate of this secondary cascade seems to be highly dependent on the solar wind streams analyzed.

We have studied the spatial properties of magnetic field fluctuations in the solar wind by using the Spatio temporal Analysis Field Fluctuation (STAFF) search coil magnetometer on board the Cluster spacecraft at 1 AU, which has a sampling frequency of 450 vec/s. The major result is that at small scales (less than the proton Larmor radius) the magnetic field does not resemble a sea of homogeneous fluctuations, but rather a two-dimensional plane containing thin current sheets and discontinuities with spatial sizes ranging from proton down to the electron scales. At the Hall Magnetohydrodynamic (MHD) scales those current sheets have been compared with those developed in a bidimensional Hall MHD simulation of freely decaying turbulence finding a good qualitative agreement of their spatial properties.

We pointed out that these isolated structures may be manifestations of intermittency that localize sites of turbulent dissipation. Studying the relationship between turbulent dissipation, reconnection, and intermittency is crucial for understanding the dynamics of laboratory and astrophysical plasmas and is matter of ongoing work.

#### Phase-syncronization and energy cascade in solar wind turbulence

The energy cascade in solar wind magnetic turbulence is investigated using 2 vec/s resolution MESSENGER data in the inner heliosphere. Our analysis of solar wind magnetic field fluctuations make a combined use of two independent techniques, namely the empirical mode decomposition (EMD) and the local intermittency measure (LIM) based on wavelet analysis. The former provides a decomposition of the solar wind turbulent fields in a limited number of modes (including information on the phase), while the latter enables the detection of intermittent structures and the energy transfer in the flow. The decomposition of magnetic field time series in intrinsic functions, each characterized by a typical time scale, reveals phase reorganization. This allows for the identification of structures of all sizes generated by the nonlinear turbulent cascade, covering both the inertial and the dispersive ranges of solar wind turbulence. The important result of the analysis is the presence of correlation (or anticorrelation) of phases between pairs of neighboring time scales, whenever localized peaks of magnetic energy are present at both scales (regardless of their amplitude), consistent with the local character of the energy transfer process. The robustness of the analysis is related to the strong correspondence between the synchronization of the phases of the modes and the occurrence of peaks of magnetic energy by applying two complete independent methods of data analysis. The next step is to study the magnetic field vector properties during the time intervals where phasesynchronization is detected in order to characterize the spatial properties of the magnetic energy cascade.

#### Data analysis and modeling of solar wind turbulence

We used single point spacecraft observations of the turbulent solar wind flow to study nonaxisymmetric anisotropy of the turbulent fluctuations in the solar wind. We used obtained results to test different phenomenological models of magnetohydrodynamic (MHD) turbulence. Using Ulysses magnetic field observations in the fast, quiet polar solar wind we find that the Goldreich-Sridhar model of MHD turbulence is not consistent with the observed anisotropy, whereas the observations are well reproduced by the "slab+2D" model. Therefore Goldreich-Sridhar model alone cannot account for the observations unless an additional component is also present.

Moreover, we studied spectral features of Alfvénic turbulence in fast solar wind. We proposed a general, instrument-independent method to estimate the uncertainty in velocity fluctuations obtained by in situ satellite observations in the solar wind. We show that when the measurement uncertainties of the velocity fluctuations are taken into account the

less energetic Elsasser spectrum obeys a unique power law scaling throughout the inertial range as prevailing theories of MHD turbulence predict. Moreover, in the solar wind interval analyzed, the two Elsasser spectra are observed to have the same scaling exponent  $\gamma = -1.54$  throughout the inertial range.

Finally, we studied dynamics of the residual energy in MHD turbulence. In situ observations of the solar wind as well as numerical simulations show that the energy of magnetic field fluctuations always exceeds that of the kinetic energy, and therefore the difference between the kinetic and magnetic energies, known as the residual energy, is always negative. We studied the dynamics of the residual energy for strong, anisotropic, critically balanced magnetohydrodynamic turbulence using the eddy damped quasi-normal Markovian approximation. Our analysis shows that for stationary critically balanced MHD turbulence, negative residual energy will always be generated by nonlinear interacting Alfvén waves. This finding offers a general explanation for the observation of negative residual energy in solar wind turbulence and in the numerical simulations.

#### Magnetic moment non-conservation in magnetohydrodynamic turbulence models

Many commonly used theories that describe particle motion in perturbed magnetic fields assume that particle magnetic moment  $\mu$  is on average constant. When magnetic moment is not conserved, the associated effects, such as particle energization, can have a bearing on astrophysical phenomena such as coronal heating, cosmic ray transport, temperature anisotropies in the solar wind and energy release by magnetic reconnection. Furthermore  $\mu$  conservation is strictly related to particle confinement in plasma machines and dynamically chaotic systems. The conditions that guarantee conservation of  $\mu$  are well understood in ideal circumstances. However the various conditions that can lead to significant levels of non-conservation remain the subject of ongoing discussion, especially in turbulent systems, with potentially major impact on understanding plasma dissipation and related topics. Using test particle simulations, we have studied magnetic moment conservation for charged particles in presence of a single electromagnetic wave as well as in presence of turbulent magnetic fields having one dimensional spectra comparable to those measured in the solar wind. We found different regimes of magnetic moment statistical behavior, related not just to the variation of the turbulence level, but also to the different time scale at which magnetic moment conservation is studied. The results provide a basic view of how magnetic moments are modified in simplified models, and in particular how magnetic moment changes are related to pitch angle changes and sampling of magnetic variations due to spatial diffusion.

#### Non diffusive propagation of solar energetic particles and distributions of magnetic variances

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. Those evidences call for an accurate investigation of the magnetic field fluctuations properties at the resonance frequencies, upstream of the shock's fronts. Normalized magnetic field variances, indeed, play a crucial role in the determination of the pitch angle scattering times and then of the transport regime. A recent analysis investigates the time behavior of the normalized variances of the magnetic field fluctuations, measured by the Ulysses spacecraft for several hours upstream of the corotating interaction region (CIR) shock, for those events which exhibit superdiffusion for energetic electrons. We find that for the events here considered exhibit, from about 10 hours to 100 hours from the shock front, a quasi-constant value for the normalized magnetic field variance. This rules out the presence of a varying diffusion coefficient and confirms the possibility of superdiffusion for energetic electrons. A statistical analysis of the scattering times for the CIRs events has also been performed; the obtained power law distributions of scattering times are in qualitative agreement with superdiffusive processes described by a Lévy random walk.

#### Particle acceleration at collisionless shocks in the case of superdiffusive propagation

In a number of studies performed in the previous years, we have shown that the transport of energetic particles and cosmic rays in the presence of magnetic turbulence can be superdiffusive rather then simply diffusive. This finding is going to influence the most popular mechanism for the acceleration of cosmic rays, which is a first order process called diffusive shock acceleration (DSA). The theory of diffusive shock acceleration is extended to the case of superdiffusive transport, i.e., when the mean square deviation grows as  $t^{\alpha}$ , with  $\alpha > 1$ . By using the propagator appropriate for Levy random walk, it is found that indices of energy spectra of particles are smaller than those obtained where a normal diffusion is envisaged, with

the spectral index decreasing with the increase of  $\alpha$ . A new scaling for the acceleration time is also found, allowing substantial shorter times than in the case of normal diffusion. Within the framework of superdiffusive shock acceleration (SSA) we can explain a number of observations of flat spectra in various astrophysical and heliospheric contexts.

#### 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 104 to 107 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 largescale magnetic field, in local approximation; while the turbulent dynamics at small scales is described by using a lowdimensional model (shell model). The model addresses questions of dynamo action threshold, magnetic field saturation, magnetic field reversals, nature of the dynamo transition and the changes of small-scale turbulence as a consequence of the dynamo onset. In particular the results of the model show that the large-scale dynamo transition displays a hysteretic behavior and therefore a subcritical nature. The model successfully reproduces magnetic polarity reversals, showing the capability to generate persistence times which are increasing for decreasing magnetic diffusivity. 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 Alfven waves. This energy is then channeled towards short scales through a turbulent cascade until it can be transfered 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). Through a massive process of optimization and parallelization of the numerical algorithm, we were able to perform simulations in 2D-3V phase space configuration and very recently in full 3D-3V configuration within a European PRACE project of high performance computing.

Moreover, the numerical hybrid Vlasov-Maxwell code has been successively updated in such a way to include the kinetic dynamics of heavy ions. Numerical simulations have been therefore performed to investigate the role of kinetic effects in a two-dimensional turbulent multi-ion plasma, composed of protons, alpha particles, and fluid electrons. In the typical conditions of the solar-wind environment, and in situations of decaying turbulence, the numerical results showed that the velocity distribution functions of both ion species depart from the typical configuration of thermal equilibrium. These non-Maxwellian features are quantified through the statistical analysis of the temperature anisotropy, for both protons and alpha particles. Both ion species manifest a preferentially perpendicular heating, although the anisotropy is more pronounced for the alpha particles, according to solar wind observations. The anisotropy of the alpha particle, moreover, is correlated to the proton anisotropy and also depends on the local differential flow between the two species. The physical phenomenology recovered in these numerical simulations reproduces very common measurements in the turbulent solar wind, suggesting that the multi-ion Vlasov model constitutes a valid approach to understanding the nature of complex

kinetic effects in astrophysical plasmas.



Figure 1: Velocity field in threedimensional Vlasov turbulence. Many vortical structures can be recognized.



Figure 2: Zoom of the magnetic field fluctuations, together with the squared total current density. A magnetic structure (3D vortex, or flux-tube) is identified.

#### 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. Using direct numerical simulations of the hybrid Vlasov-Maxwell model, kinetic processes are investigated m in a two-dimensional turbulent plasma. In the turbulent regime, kinetic effects manifest through a deformation of the ion distribution function, mainly manifesting through the generation of temperature anisotropy regions. These patterns of non-Maxwellian features are concentrated in space nearby regions of strong magnetic activity: the distribution function is modulated by the magnetic topology, and can elongate along or across the local magnetic field. In particular, temperature anisotropy and distortions are concentrated near coherent structures, generated as the result of the turbulent cascade, such as current sheets, which are nonuniformly distributed in space. Here, the partial variance of increments (PVI) method has been employed to identify high magnetic stress regions within a two-dimensional turbulent pattern. Conditional sampling methods employing the PVI method, applied in solar wind observational studies, suggest that the largest and most important distortions of the proton distribution function occur in the immediate vicinity of discontinuities and not in the smoothest regions. The statistical analysis provides strong evidence that coherent structures are connected to enhanced distortions of the distribution function, but also suggest that there exists a hierarchy of current sheet intensities, where the most intense are associated with the most non-homogeneous kinetic effects, as recently shown in solar wind.

#### 1.2 OBSERVATIONS AND TURBULENCE MODELS IN THE SOLAR ATMOSPHERE

#### Low Dimensional Solar Dynamo Model

A new low dimensional model for Solar Dynamo is built recently in order to interpret the presence of time scales (QBO) smaller than the predominant period of 11 years, as due to a nonlinear coupling of the magnetic field with a time dependent OMEGA effect. The latter is described by the evolution of the zonal shear, dynamically integrated with the induction equation. The model is built up retaining the main physical ingredients concurring to the dynamo effect by modeling the equations in terms of sources and sinks. In this way, a low order ALPHA<sup>2</sup>-OMEGA dynamo model is obtained and then numerically solved. The results show an oscillatory behavior of the magnetic field components reproducing a basic cycle and superimposed characteristic smaller timescales different from the frequency of the source terms. Moreover, a double-peaked structure has been found during the maxima of the magnetic field strength, resembling the behavior of the solar activity as seems to be revealed by several solar cycle indicators. A phase shift between the poloidal and toroidal magnetic field components is also obtained.

#### 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 spatiotemporal 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° and +25° 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.

#### Small scale and discontinuity generation in open-field line regions of the solar Corona

Alfvénic fluctuations are commonly detected in the solar wind. Recently, evidences of the presence of Alfvén waves in the solar corona have been revealed. Open-field line regions, like coronal holes, are dominated by a sigle magnetic polarity, but small regions of the opposite polarity are present in photospheric magnetograms. We built a model for the magnetic field above such mixed-polatity regions; the model corresponds to a complex 3D potential magnetic field, where several spatial scales are present. The propagation of Alfvén waves through such an inhomogeneus structure is studied by means of a WKB approach. We found that small scales at relatively low altitudes (ten megameters) above the coronal base, forming a power law spectrum. The slope (about -2) is steeper than in MHD turbulence; however is could represent a seed for a subsequent faster fomation of a turbulence due to nonlinear coupling at higher altitudes. The presence of separatrices in the magnetic structure leads to the formation of discontinuities in the wave profile, which are rotational discontinuities propagating quasi-perpendicularly to the ambient magnetic field. These structures propagates upwards reaching the solar wind. Thus, they can represent a fraction of discontinuities commonly detected in the interplanetary medium.

#### Ion beams in the Earth's magnetotail: resonant acceleration versus stochastic acceleration

Ion beams with energies of the order of several tens of keV are frequently observed in the Earth's magnetotail. In the Earth plasma sheet boundary layer two types of ion beams (so-called beamlets of type I and of type II) were investigated for more then two decades. Type I beamlets have energies < 20 keV and small velocity dispersion, while type II beamlets have energies up to 100 keV and large velocity dispersion. It is believed that beamlets of type I result from non-adiabatic and resonant acceleration by the cross-tail electric field  $E_y$  at the fulfillment of the resonant condition in the current sheet, while beamlets type II could be generated by sufficiently large level of electromagnetic fluctuations in the magnetotail. The resonant condition is very sensitive to the presence of the perturbation and eventually should be destroyed by growing "noise". We performed test particle simulation taking into account two possible acceleration mechanisms, cross-tail electric field Ey and stochastic acceleration due to electromagnetic perturbations. Electromagnetic perturbation were generated by a set of oscillating clouds in the plasma sheet. We obtained that type I beamlets could be observed even in the presence of moderate levels of perturbation  $\delta B = B_z(z=0)$ , where  $B_z$  is a magnetic field component perpendicular to the current sheet plane. Increasing the perturbation level, beamlets of higher energy are obtained but energies are no more discrete. The interplay of ion resonant acceleration and magnetic perturbation in the magnetotail leads to a continuous transition from beamlets of type I to beamlets of type II. A comparison of the numerical results with the observation of ion populations in magnetotail is also discussed.

#### 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. It is found that the heavy ion energy gain is larger than mass proportional, so that this effect can explain the observations.

#### Turbulent pair dispersion 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. We have used observations of solar granulation obtained with the New Solar Telescope of Big Bear Solar Observatory to study the turbulent pair dispersion of photospheric bright points in a quiet-Sun area, a coronal hole, and an active region plage. In all the three magnetic environments, it is found that the pair mean-squared separation  $\Delta^2(t)$  follows a power-law timescaling  $\Delta^2(t) = t^{\eta}$  in the range 10 s < t < 400 s. The power-law index is found to be  $\eta = 1.5$  for all the three investigated regions. We have shown that these results can be explained in the same framework as the classical Batchelor theory, under the hypothesis that the observed range of timescales corresponds to a non-asymptotic regime in which the photospheric bright points keep the memory of their initial separations.

#### **1.3 MAGNETOSPHERIC PHENOMENA AND GEOPHYSICS**

#### 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 us 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 cvcle. 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 phaseshift 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. We also focused on the investigation of trends from the 1167 USA stations. We found strong evidence that more than 50 percent of the analized USA stations experiences a significant trend over the last century. Our spatio-temporal analysis reveals a significant cooling trend in the South-East and significant warming trends in the rest of the contiguous US thus showing the complex spatio-temporal evolution of climate change at local scales.

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

We investigated how tsunamis, generated as a consequence of large earthquakes, modify the main tidal components in the Mediterranean sea. We find two kinds of transient signatures which can be attributed to the destabilizing effect of the tsunami on the main tidal components: 1) the excitation of a broad spectrum of frequency fluctuations, superimposed to the diurnal and semidiurnal tidal components, 2) the phase delay of the long term astronomical component of the tide.

#### 1.4 LABORATORY PLASMAS

#### Turbulence in pure electron plasmas

Electron plasmas confined in Penning-Malmberg traps evolve, in a wide range of operational parameters, as nearideal 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 experimental results have been analyzed by means of wavelet transforms and Proper Orthogonal Decomposition (POD). The wavelet analysis shows that most of the enstrophy is contained at spatial scales corresponding to the typical size of the persistent vortices in the 2D electron plasma flow. The POD analysis allows one to identify the coherent structures which give the dominant contribution to the plasma evolution. The statistical properties of the turbulence have been investigated by means of Probability Density Functions (PDFs) and structure functions of spatial vorticity increments. The analysis evidences how the shape and evolution of the dominant coherent structures and the intermittency properties of the turbulence strongly depend on the initial conditions for the electron density.

#### Non-neutral complex plasmas

A plasma of particles with the same sign of charge, can be easily confined under ultra-high vacuum conditions in Penning-Malmberg traps, where the time evolution of the system is monitored for very long times by means of electrostatic and optical diagnostic systems. Complex (dusty) plasmas are ionized gases that contain a distribution of micrometer-sized particles with a surface charge of the order of a few thousand electron charges. The interplay between a wide range of scales in time and space gives rise to new characteristic physical phenomena. Laboratory complex plasmas generally satisfy a global (quasi-)neutrality condition. A different concept is represented by a non-neutral complex plasma. To investigate the dynamics of this system, the DuEl (Dust-Electron) device, a modified Penning-Malmberg trap for the confinement of dustcontaminated electron plasmas, is currently under development at the University of Milano. The experimental set-up will include a dust injection system and a Penning-Malmberg trap for the confinement of the dust-contaminated electron plasma. To support the experimental project, a two-dimensional 'hybrid' Particle-In-Cell code has been built-up to simulate the transverse dynamics of such plasmas and support the experimental work. A kinetic description is adopted for the dynamics of the dust component, including gravity effects, while a mass-less fluid approximation (drift-Poisson) is exploited for the electron population. A polar cylindrical mesh is used and the Fast Fourier Transform technique is applied in the theta direction to solve the Poisson equation. Numerical simulations with different initial conditions for the electrons and the dust are performed to study the influence of the dust on the fluid (Kelvin-Helmholtz) instabilities developing in the electron plasmas. The implementation of other characteristic phenomena of interest, e.g. residual gas friction and dust charge fluctuations, is also under development.

#### Kinetic evolution of high frequency plasma waves in Penning-Malmberg traps

A collection of particles with the same sign of charge is usually referred to as a nonneutral plasma. These unneutralized gases can be confined in experimental devices called Pennig-Malmberg traps, in which the confined gas assumes a cylindrical shape. The reason why the term "plasma" has been first used for this kind of systems principally lyes on the fact that they exhibit many of the collective phenomena that are usually typical features of ordinary neutral plasmas. For these reasons, experiments with nonneutral plasmas represent an indispensable tool to investigate basic processes in plasma physics, like, for example, the collisionless Landau damping of electrostatic waves and the linear and nonlinear regime of wave-particle interaction. When a plasma has a finite radial geometry, electrostatic plasma waves can propagate at frequency smaller than the plasma frequency; these waves are usually called Trivelpiece-Gould (TG) waves. The kinetic

dynamics of a column of plasma with a single sign of charge confined in a Penning-Malmberg trap can be described through the drift-kinetic equations. Through a very active collaboration with the nonneutral plasma physics group of the University of California at San Diego, we started a novel line of research focused on the systematic comparison between experimental and numerical results concerning the excitation, the propagation and the stability of the TG modes, both in linear and in the nonlinear regime. In the last two years we developed numerical codes in different configuration that integrate selfconsistently the drift-kinetic equation coupled to Poisson's equation thus properly describing the kinetic dynamics of pure ion (or pure electron) plasmas. Moreover, very recently, the effects of collisions have been added into the numerical calculation through the implementation of diffusive collisional operators of the Fokker-Planck type.

#### A PUBLICATIONS ON SCIENTIFIC JOURNALS

#### A.1 Publications on international journals

#### A.1.1 Publications on international journals printed in 2012

- 1. Servidio A., Valentini F., Califano F., Veltri P., Local kinetic effects in two-dimensional plasma turbulence Physical Review Letters, **108**, 045001 (2012).
- Onofri M., Vecchio A., De Masi G., Veltri P., *Propagation of gravity waves in a convective layer* The Astrophysical Journal, 746, 58-65 (2012).
- 3. Greco A., Matthaeus W.H., D'Amicis R., Servidio S., Dmitruk P., *Evindence for nonlinear development of magnetohydrodynamic scale intermittency in the inner heliosphere* The Astrophysical Journal, **749**, 1-9 (2012).
- Wan M., Oughton S., Servidio S., Matthaeus W. H., von Kármán self-preservation hypothesis for magnetohydrodynamic turbulence and its consequences for universality Journal of Fluid Mechanics, 697, 296-315 (2012).
- Matthaeus, W. H., Servidio S., Dmitruk P., Carbone V., Oughton S., Wan M., Osman K. T., Local anisotropy, higher order statistics, and turbulence spectra The Astrophysical Journal, 705, 103 (2012).
- Vecchio A., Laurenza M., Meduri D., Carbone V., Storini M., *The dynamics of the solar magnetic field: polarity reversals, butterfly diagram and quasi-biennial oscillations* The Astrophysical Journal, 749, 27 (2012).
- Laurenza M., Vecchio A., Carbone V., Storini M., *Quasi Biennial Modulation of Galactic Cosmic Rays* The Astrophysical Journal, 749, 167 (2012).
- Vecchio A., Anzidei M., Capparelli V., Carbone V., Guerra I., Has the Mediterranean sea felt the March 11th, 2011, Mw 9.0 Tohoku-oki earthquake? Europhysics Letters, 98, 59001 (2012).
- Dalena S., Chuychai P., Mace R. L., Greco A., Qin G., Matthaeus W. H., Streamline generation code for particle dynamics description in numerical models of turbulence Computer Physics Communications, 183, 1974-1985 (2012).
- Dalena S, Greco A., Rappazzo A. F., Mace R. L., Matthaeus W. H., Magnetic moment nonconservation in magnetohydrodynamic turbulence models Physical Review E, 86, 016402-1 (2012).
- Valentini F., Perrone D., Califano F., Pegoraro F., Veltri P., Morrison P. J., O'Neil T. M., Undamped electrostatic plasma waves Physics of Plasmas, 19, 092103 (2012).
- Lepreti F., Carbone V., Abramenko V., Yurchyshyn V., Goode P. R., Capparelli V., Vecchio A., *Turbulent Pair Dispersion of Photospheric Bright Points* Astrophysical Journal Letters, **759**, L17-1 (2012).
- Greco A., Valentini F., Servidio S., Matthaeus W. H., *Inhomogeneous kinetic effects related to intermittent magnetic discontinuities* Physical Review E, 86, 066405 (2012).

- Perri S., Carbone V., Vecchio A., Bruno R., Korth H., Zurbuchen T. H., Sorriso-Valvo L., *Phase-synchronization, energy cascade and intermittency in the solar wind turbulence* Physical Review Letters, 109, 1-5 (2012).
- Perri S., Zimbardo G., *Superdiffusive shock acceleration* The Astrophysica Journal, **750**, 87-91 (2012).
- Perri S., Zimbardo G., Magnetic variances and pitch angle scattering times upstream of interplanetary shocks The Astrophysical Journal, 754, 8-14 (2012).
- Perri S., Carbone V., Comment on "Effect of current sheets on the solar wind magnetic field power spectrum from the Ulysses observation: from Kraichnan to Kolmogorov scaling Physical Review Letters, 108, 1 (2012).
- Perri S., Goldstein M. L., Dorelli J. C., Sahraoui F., Detection of small-scale structures in the dissipation regime of solar-wind turbulence Physical Review Letters, 109, 1-5 (2012).
- Malara F., Nigro G., Veltri P., Onofri M., *Alfvén waves: coherent phenomena in coronal loops and open-field regions* Space Science Review, **172**, 157-167 (2012).
- Vecchio A., Laurenza M., Carbone V., Storini M., New insights on cosmic ray modulation through a joint use of non-stationary data processing methods Advances in Astronomy, article ID: 834247 (2012).
- Nisticò G., Zimbardo G., Heating heavy ions in the polar corona by collisionless shocks: a one-dimensional simulation Advances in Space Research, 49, 408-415 (2012)
- 22. Zimbardo G., Perri S., Pommois P., Veltri P., *Anomalous Particle Transport in the Heliosphere* Advances in Space Research, **49**, 1633-1642 (2012)
- Aburjania G. D., Zimbardo G., Kharshiladze O. A., *Effect of the shear flow in the generation and self-organization of internal gravity wave structures in the dissipative ionosphere* Plasma Physics Reports, 38, 972-990 (2012).
- Matthaeus W. H., Montgomery D. C., Wan M., Servidio S., *A review of relaxation and structure in some turbulent plasmas: magnetohydrodynamics and related models* Journal of Turbulence, 13, 1 (2012).
- Rappazzo F., Matthaeus W. H., Ruffolo D., Servidio S., Velli M., Interchange Reconnection in a Turbulent Corona Astrophysical Journal Letters, 758, L14 (2012).
- Donato S., Servidio S., Dmitruk P., Carbone V., Shay M. A., Cassak P. A., Matthaeus W. H., *Reconnection events in two-dimensional Hall magnetohydrodynamic turbulence* Physics of Plasmas, 19, 092307 (2012).
- 27. G. Gogoberidze, S.C. Chapman, B. Hnat, *Generation of residual energy in the turbulent solar wind* Physics of Plasmas, **19**, 102310, (2012).

- G. Gogoberidze, S.C. Chapman, B. Hnat, M.W. Dunlop, *Impact of observational uncertainties on universal scaling of MHD turbulence* Montly Notices of the Royal Astronomical Society, 426, 951 (2012).
- A.J. Turner, G. Gogoberidze, S.C. Chapman, Nonaxisymmetric Anisotropy of Solar Wind Turbulence as a Direct Test for the Models of Magnetohydrodynamic Tubulence Physical Review. Letters, 108, 085001 (2012).

#### A.1.2 Publications on international journals accepted in 2012

- 1. Capparelli V., Vecchio A., Carbone V., *Empirical mode decomposition detects a phase shifti of seasonal oscillation* to appear on Advances in Adaptive data analysis.
- Vecchio A., Laurenza M., D'Alessi L., Carbone V., Storini M., *The Empirical Mode Decomposition to study the quasi-biennial modulation of solar magnetic activity and solar neutrino flux* to appear on Advances in Adaptive data analysis
- 3. Malara F., *Alfvén waves in coronal holes: formation of discontinuities in inhomogeneous magnetic fields* to appear on Astronomy and Astrophysics
- Nigro G., Magnetic dynamo, Turbulent alpha dynamo effect, Turbulence, Magnetohydrodynamic shell model to appear on Geophysical & Astrophysical Fluid Dynamics

# **B** PUBLICATIONS ON CONFERENCE PROCEEDINGS

# **B.1** Publications on international conference proceedings in 2012

- Maero G., Cavaliere F., Cavenago M., Ikram M., Lepreti F., Paroli B., Pozzoli R., Romé M., *DuEl: A set-up for the study of non-neutral complex plasmas* 39th EPS Conference on Plasma Physics - 16th International Congress on Plasma Physics, Ratynskaia S., Blomberg L., Fasoli A. Eds., European Physical Society, p1.139 (2012)
- Lepreti F., Romé M., Pozzoli R., Vecchio A., Carbone V., Maero G., Paroli B., *Dynamical and statistical properties of two-dimensional turbulence in pure electron plasmas*  39th EPS Conference on Plasma Physics - 16th International Congress on Plasma Physics, Ratynskaia S., Blomberg L., Fasoli A. Eds., European Physical Society, p1.179 (2012)
- Trotta E. M., Zimbardo G., *Non diffusive propagation of solar energetic particles: data analysis and numerical simulations* European Conference on Laboratory Astrophysics, EDP Sciences - EAS Publications Series, pp. 99-102 (2012).

## C BOOK CHAPTERS

- Greco A., Valentini F., Servidio S., Small Scale Processes in the Solar Wind, in "Exploring the Solar Wind", M. Lazar Ed., Intech, Croatia, pp. 195-219 (2012).
- 2. Zimbardo G., Perri S.,

Superdiffusive Transport at Shocks in Space Plasmas, in "Multi-scale Dynamical Processes in Space and Astrophysical Plasmas", Leubner M. P., Voeroes Z. Eds., Springer, pp. 153-158 (2012).

#### **D** INVITED PRESENTATIONS

#### D1. Invited presentations at international conferences in 2012

 Perrone D., Valentini F., Servidio S., Dalena S., Veltri P., *Turbulence in two-dimensional multi-ions plasma: hybrid Vlasov numerical simulations* Workshop of the International Space Science Institute (ISSI): Microphysics of Cosmic Plasmas, Bern – Switzerland, April 16-20, 2012.

2. Valentini F.,

*Vlasov equation: theory and simulation* First European School on: Fundamental processes in Space Weather: a challenge in numerical modeling, Spineto, Italy, June 4-9, 2012.

3. Greco A.,

Detection and analysis of turbulent structures using the Partial Variance of Increments method Turbulent cascade in the solar wind: anisotropy and dissipation, Meudon, France, September 17-21, 2012.

- 4. Zimbardo G., Perri S., Superdiffusive transport in space plasmas and superdiffusive particle acceleration at shocks ISSI workshop on Microphysics of Cosmic Plasmas, Bern, Switzerland, April 16-20, 2012.
- 5. Zimbardo G., Perri S.,

*Superdiffusive propagation in space plasmas: numerical simulations and experimental evidences* European Geosciences Union general assembly 2012, Vienna. Austria, April 22-27, 2012.

6. Zimbardo G.,

Non-diffusive transport in space and laboratory plasmas Internatioal School of Space Science, 2012 Course on "Astrophysical and Space Plasmas", L'Aquila, Italy, September 2-8, 2012.

7. Zimbardo G.,

*The Heliosphere: the interactions of the solar wind with the interstellar medium* Internatioal School of Space Science, 2012 Course on "Astrophysical and Space Plasmas", L'Aquila, Italy, September 2-8, 2012.

- Nigro G., Carbone V., Primavera L., Zonal Shear in a Solar Dynamo Model 2012 AGU Fall Meeting, San Francisco, USA, December 3-7, 2012.
- Servidio S., Dmitruk P., Valentini F., Greco A., Veltri P., Carbone V., Donato S., Wan M., Shay M., Cassak P., Matthaeus W. H., Overview on numerical studies of reconnection and dissipation in the solar wind Solar Wind 13, Kona-Kailua, Big Island, Hawaii, USA, June 18-22, 2012.
- Servidio S., Dmitruk P., Valentini F., Greco A., Veltri P., Carbone V., Donato S., Wan M., Shay M., Cassak P., Matthaeus W. H., Magnetic Reconnection in a Turbulent Environment Solar Heliospheric & Interplanetary Environment (SHINE), Wailea Maui, Hawaii, USA, June 25-29, 2012.
- Servidio S., Valentini F., Califano F., Veltri P., Local kinetic effects in a turbulent plasma: numerical simulations 2012 AGU Fall Meeting, San Francisco, USA, December 3-7, 2012.
- 12. Perri S., Goldstein M. L., Dorelli J. C., Sahraoui F.,

Detection of magnetic discontinuities in the dissipation regime of solar wind turbulence 2012 AGU Fall Meeting, San Francisco, USA, December 3-7, 2012.

#### D2. Invited presentations at national conferences in 2012

 Valentini F., Perrone D., Califano F., Pegoraro F., Veltri P., Morrison P. J., O'Neil T. M., Undamped electrostatic plasma waves: theory and Vlasov simulations XCVIII Congresso Nazionale, Società Italian di Fisica, Naples, Italy, September 17-21, 2012.

#### **E PRESENTATIONS AT CONFERENCES**

#### E1. Presentations at international conferences in 2012

- Perrone D., Valentini F., Servidio S., Dalena S., Veltri P., Study of kinetic effects in turbulent plasma in presence of alpha particles First European School on: Fundamental processes in Space Weather: a challenge in numerical modeling, Spineto, Italy, June 4-9, 2012.
- Valentini F., Perrone D., Califano F., Pegoraro F., Veltri P., Morrison P. J., O'Neil T. M., Undamped electrostatic plasma waves
   54th Annual Meeting of the APS Division of Plasma Physics, Providence, Rhode Island, USA, October 29 – Novermber 2, 2012.
- 3. Valentini F., *Kinetic simulations of plasma turbulence in the solar wind: temperature anisotropy of the ion species* Arcetri 2012 Workshop on Plasma Astrophysics, Arcetri, Italy, November 5-8, 2012.
- Maero G., Cavaliere F., Cavenago M., Ikram M., Lepreti F., Paroli B., Pozzoli R., Romé M., DuEl: A set-up for the study of non-neutral complex plasmas 39th European Physical Society Conference on Plasma Physics - 16th International Congress on Plasma Physics, Stockholm, Sweden, July 2-16, 2012.
- Lepreti F., Romé M., Pozzoli R., Vecchio A., Carbone V., Maero G., Paroli B., Dynamical and statistical properties of two-dimensional turbulence in pure electron plasmas 39th European Physical Society Conference on Plasma Physics - 16th International Congress on Plasma Physics, Stockholm, Sweden, July 2-16, 2012.
- Romé M., Lepreti F., Maero G., Pozzoli R., Vecchio A., Carbone V., *Analysis of the two-dimensional turbulence in pure electron plasmas by means of advanced statistical techniques*  NON-NEUTRAL PLASMA PHYSICS VIII: 10th International Workshop on Non-Neutral Plasmas, Greifswald, Germany, August 27-30, 2012.
- Romé M., Cavaliere F., Cavenago M., Ikram M., Lepreti F., Maero G., Paroli B., Pozzoli R., *Experimental and numerical investigation of non-neutral complex plasmas* NON-NEUTRAL PLASMA PHYSICS VIII: 10th International Workshop on Non-Neutral Plasmas, Greifswald, Germany, August 27-30, 2012.
- Zimbardo G., Perri S., Superdiffusive Shock Acceleration Arcetri 2012 Workshop on Plasma Astrophysics, Arcetri, Italy, November 5-8, 2012.
- Perri S., Zimbardo G., Superdiffusive shock acceleration European Geosciences Union general assembly, Wien, Austria, April 22-27, 2012.
- 10. Dolgonosov, M., Zelenyi, L., Zimbardo, G., Perri, S., Kovrazhkin, R.,
*Could we use beamlets as a tool for remote sensing of the magnetotail?* 39th COSPAR Scientific Assembly, Mysore, India, July 14-22, 2012.

- Carbone V., Servidio S., Vecchio A., Anzidei M., Guerra I., *Possible tsunami transmission across the Strait of Gibraltar: numerical simulations* AGU Fall Meeting, San Francisco, USA, December 3-7, 2012.
- Matthaeus W. H., Servidio S., Dmitruk P., Carbone V., Oughton S., Wan M., Osman K. T., Local anisotropy and power spectra in magnetohydrodynamic turbulence AGU Fall Meeting, San Francisco, USA, December 3-7, 2012.
- Servidio S., Matthaeus W. H., Dmitruk P., Rappazzo F., Oughton S., Wan M., Ruffolo D. J., Magnetic flux surfaces in anisotropic threedimensional complex fields AGU Fall Meeting, San Francisco, USA, December 3-7, 2012.
- Servidio S., Valentini F., Califano F., Veltri P., *Kinetic effects in two-dimensional plasma turbulence* Arcetri 2012 Workshop on Plasma Astrophysics, Arcetri, Italy, November 5-8, 2012.
- Perri S., Carbone V., Vecchio A., Bruno R., Korth H., Zurbuchen T. H., Sorriso-Valvo L., *Energy cascade and phase syncronization in the solar wind turbulence* SHINE, Maui, Hawaii, June 25-29, 2012.
- Perri S., Goldstein M. L., Dorelli J. C., Sahraoui F., Detection of small-scale structures in the dissipation regime of solar-wind turbulence SHINE, Maui, Hawaii, June 25-29, 2012.

#### E1. Presentations at national conferences in 2012

 Perri S., Zimbardo G., Superdiffusive shock acceleration XCVIII Congresso Nazionale della Societa' Italiana di Fisica, Naples, Italy, September 16-22, 2012.

## 2. BIOMEDICAL PHYSICS

Professors and researchers:	L. Sportelli (Molecular Biophysics Group, University of Calabria) A. Santaniello (Biomedical Physics, University of Calabria)
Undergraduate students:	I. Bonetti
Collaborators:	E. Marsich (Life Science Department, University of Trieste) I. Nicotera (Chemistry Department, University of Calabria)

**Research subjects:** 

1. Dosimetry with innovative EPR-sensitive materials

2. Study of radiation effects in biomolecules of dosimetric interest

#### Introduction

Innovative radiotherapeutic methods conform the therapeutic radiation beam to the shape of the tumor, which improves dose delivery to the patient as compared with conventional radiotherapy since a higher dose of radiation reaches the tumor with respect to that to the surrounding normal tissues. The combined good tumor control and reduced toxicity of the radiation thus achieved avoids tumor recurrence while sparing critical organs: the quality of life of the treated patient is improved and, additionally, collateral sanitary treatments are limited.

As a practical drawback, the strong field gradients used in these treatments are challenging for dosimetry, and the accurate positioning of the patient, image-controlled by specialized software, has to match a correspondingly accurate dosimetric determination, in order to achieve an effective treatment. Research in the field aims to improve the detection limit and the dynamic range of the dosimeters, and the spatial resolution of the dose measurements. For this purpose, innovative dosimetric materials are synthesized, their dosimetric features are characterized, and new dosimetric approaches are developed.

#### 2.1 DOSIMETRY WITH INNOVATIVE EPR-SENSITIVE MATERIALS

#### 2.1.1 New approaches: HAp-alginate dosimetry

A patent is applied for HAp-alginate EPR dosimetry, in collaboration with Dr. E. Marsich of the Life Science Department of the University of Trieste. Hydroxyapatite-alginate (Hap-Al) is a synthetic, low-density, biocompatible composite material of recent synthesis, which we showed to present stable radioinduced radicals.

#### 2.1.2 Dosimetric characterisation of newly synthesised EPR-sensitive materials

Clinical protocols indicate EPR dosimetry based on alanine as the radiosensitive material for the high dose determinations (above 10 Gy), i.e., EPR dosimetry is precluded to both the most common radiotherapeutic schemes, in which the total dose is fractionate in steps of the order of 2 Gy, and modern radioterapeuthic approaches, in which the dynamic range of the dose determination is wide. Alanine dosimeters do not garantee, for doses lower than 10 Gy, the very low uncertainties required clinically (below 5%). This is the consequence of a combination of high detection limit, low sensitivity, and dependence on the preparation batch. Formates, a class of metallic salts of the formic acid, might represent an alternative to alanine because they present, separately or in combination, a low detection limit, a simple line-shape, a fair independence on the preparation batch and a high sensitivity, especially if modified by doping with transition metal atoms.

We synthesised for the first time Zn and Cd-doped  $HCO_2LiH_2O$  (Li-formate) dosimeters, by recrystallization from a water solution of Li-formate and a salt containing the metallic doping species. Part of this work was performed within a "Tesi Magistrale" of the Department (by I. Bonetti). Small pellets (with a linear size of the order of a few mm) were prepared by using an ordinary mechanical press (die size of the order of 1 cm) by using an especially developed procedure.

Preliminary irradiation of the dosimetric materials was performed with orthovoltage beams from a laboratory equipment (X-ray irradiator source Faxitron 650X, typical energy: 100 keV) at the Molecular Biophysics Laboratory. The calibration curves of Zn and Cd-doped formates were obtained in a dose interval of clinical interest (approximately 1-100 Gy) for selected mass concentrations of the doping species. A linear dose dependence was observed in the studied interval (see Fig.1).



Fig.1 Signal versus exposure time of Zn, Cd and Ni-doped Li-formates as obtained for selected mass content of the doping species. Pure Li-formate and alanine curves are also shown for comparison. Lines are drawn as a help for the eyes.

The figure reports, for each sample, the measurements taken within the first hour from irradiation (see next session for a discussion of the temporal dependence of the signal). The data obtained for a Ni-doped sample, un-doped Li-formate and alanine are also shown for comparison purposes. Our results indicate a signal larger than that of alanine and of the pure formate for all doped samples, with sensitivities (as measured by the slope of the linear fit to the data) from about 2 to about 4 times larger than that of alanine.

#### 2.2 STUDY OF RADIATION EFFECTS IN BIOMOLECULES OF DOSIMETRIC INTEREST

#### 2.2.1 Synthesis and EPR studies of transition metal ions doped Li-formates

Formates are possible alternative materials to alanine, for both the clinical applications of EPR dosimetry at low doses, and the realization of very small EPR dosimeters (of the order of a few mm). In particular, literature studies indicate that the low dose performance of Li-formate can be improved by inclusion of paramagnetic species like Ni atoms, which increases the sensitivity by a factor of the order of two with respect to the undoped material. Radiation effects in these materials are currently under study, in order to achieve optimal dosimetric performances. We studied Li-formate modified by the inclusion of the species Zn, Cd, and Ni at different mass concentrations. The samples were synthesised by recrystallisation from water solutions of Li-formate and salts of the doping metal, irradiated at orthovoltage beam energies (100 keV), and clinically relevant dose values (from about 1 to about 100 Gy) at the Molecular Biophysics Laboratory.

The EPR signal intensity depends on the metal atom concentration (see Fig. 2), reaching a maximum for mass concentration values of about 1-2% with Zn, and an intensity value in agreement with literature results with Ni-doped Liformate (wt =1.6%, not shown).



Fig. 2 Sensitivity increase upon doping with metal atoms, as measured by the peak-to-peak intensity of the EPR radioinduced signal, as a function of the mass concentration of the dopant atom in water solution of Li-formate and the

metal salt used as dopant compound. The corresponding EPR spectra were measured immediately after exposure for 1 h to 100 keV photons.

No maximum is visible up to 2.5% of Cd doped Li-formate.

Residual humidity, coming from not extensively dryed samples, plays an important role, influencing the time behaviour of the radioinduced signal of each sample (not shown). This was clearly demonstrated by measuring at different time intervals the EPR signal of a pure Li-formate sample recrystallised from a water solution. Our findings corroborate recent literature data, which revealed an unexpected dependence of the EPR signal of pure Li-formate on ambient humidity.

The present results confirm larger signals with respect to both alanine and the native formate for all studied samples, allowing, in principle, the preparation of miniaturised pellets (3-4 mm linear size) to be used for the dosimetry of spatially dishomogeneous fields. The study of the dependence of the dosimetric signal of the doped compound on the residual water content clarifies that special preparation procedures need to be developed in order to obtain a controlled water content and, correspondingly, a controlled dosimetric signal.

#### 2.2.2 Radioinduced modifications of carbohydrates: the dependence on ambient humidity

Sugars are very sensitive EPR dosimetric materials used for retrospective dosimetry, e.g., emergence dosimetry of radiation accidents or other un-programmed exposures, because of their ubiquitous presence in households and working environments. Sugars might be interesting for medical dosimetry as well, because of their high sensitivity and low detection limit (doses as low as 0.5 Gy can be determined), but their complex, time-dependent radioinduced EPR spectrum, resulting from several radicals not yet fully assigned, at present prevents them from clinical use. Besides this, sugars are hygroscopic. In particular, sucrose powder is known to cake, i.e., to form aggregates of crystals, giving rise to four different sugar-water phases depending on relative humidity values, temperature and crystal size. Ambient humidity is known to influence the intensity of the EPR signal of several dosimetric materials, concurring to rise the total uncertainties of the dose evaluation above 5%, the limit value admitted by the radiotherapeutical dosimetric protocols. Besides this, the detailed interpretation of the EPR spectra including several free-radicals, as in case of sugars, might be complicated by a specific dependence of the radical species on water content.

We prepared caked sucrose at room temperature, under controlled conditions corresponding to relative humidity values in the ambient range (Hr = 33%, 43%, 75%, 84% and 97%), by exposing the sucrose powder for several days to a saturated solution of an appropriate salt. Different grain sizes were used (average values: 80, 250, 500  $\mu$ m). Correspondingly, phases B, C and D were obtained. In the case of phases B and C, small amounts of water are absorbed according to the funicular scheme (permanent contact among particles by liquid capillary bridges, and sparse liquid-filled pores) or the capillary one (lumping of all particles by capillary forces, all pores filled by the liquid with no dissolution of the particles), respectively. Phase D is a slurry (syrup), in which the grains are freely dispersed in a continuous liquid medium. At room temperature (our investigation), the onset of each phase is known to shift towards lower values of the relative humidity if the grains are smaller. The caking phases were measured by NMR (Laboratory PCSM - "M. Terenzi", Chemistry Department - UNICAL). Phases B and C showed a negligible proton signal below Hr = 84% and a weak, but clear contribution, at the relative humidity value of Hr = 84%. For the syrup phase D observed for Hr = 97%, the diffusion coefficients of free water and proton relaxation times were determined. We studied by EPR the funicular phase B and the capillary phase C. The EPR signal was radioinduced, as before, by orthovoltage beams (100 keV) at a nominal dose of 157 Gy and the spectra were measured immediately after irradiation, few days later, and several months afterwards, in order to study the time evolution and stability of the radical species. The samples were kept sealed over the full time period.

The shape of the EPR sucrose signal for Hr = 75% and 84% is reported in Fig.3, as measured few days after irradiation, i.e., when the unstable radicals observed immediately after irradiation have decayed. The signal is arbitrarily normalized to the positive maximum, and shifted along the B field axis in order to align to the maxima.



Fig. 3 The shape of the sucrose signal for values of the relative humidity Hr = 75% and 85%, as measured few days after irradiation, i.e., when the unstable radicals observed immediately after irradiation have decayed, and 4 months later, in order to separate permanent spectral modifications induced by water (at the lowest and highest magnetic field values) from late signal decay (in the central part of the spectra).

The weak but reproducible changes observed at the lowest and highest magnetic field values after 4 months from irradiation (Fig. 3, left panel), are already present in the spectra measured few days after irradiation (Fig. 3, right panel). The changes are associated to water-induced modifications of the spin states. The central part of the spectrum is still evolving within the first 4 months from irradiation for both Hr = 75% (see Fig. 3, right panel), and Hr = 85% (not shown). Comparison with the left panel of Fig.3 demonstrates that these "late" features evolve towards different levels of spin states for the two water contents.

According to literature data, the sucrose dosimetric signal, as measured from the peak-to-peak signal from the highest positive to the lowest negative spectral features (the *dosimetric peaks*), is mostly determined by three main radicals, each corresponding to an unpaired spin state on a C-ring atom. The resonances at the lowest and the highest magnetic field values are, instead, associated to minor radicals, not yet assigned. The minor radicals also influence the central part of the spectrum, between the dosimetric peaks. Sugar radicals are influenced by next-neighbor interactions in dry, crystalline sugars, as shown by recent comparison of double-resonance EPR (ELDOR) measurements on sugar single crystals and density functional theory (DFT) calculations on sugar clusters. Our measurements confirm the presence of a residual, very slow time decay signal in the humid powder samples for the structures near the magnetic field value of B = 3320 Gauss. These signal variations are not further affected by humidity (see Fig. 3). However, the results also indicate a different water sensitivity of the distinct radical species. This contributes to clarify the role of next-neighbor interactions in sucrose, and distinctive features of the different radical species.

## PUBLICATIONS and PRESENTATIONS

Postponed because of patent pending.

## **3. CONDENSED MATTER PHYSICS**

	Professors and Researchers	Assunta Bonanno
	110,000,000,0	Michele Camarca
		Lorenzo Salvatore Caputi
		Anna Cupolillo
		Giovanni Falcone
		Daniela Pacile Marco Papagno
		Franco Piperno
		Francesco Plastina
		Pierfrancesco Riccardi
		Antonello Sindona
		Fang Xu
Pos	Postdoc fellows	Marianna Barberio
		Pasquale Barone
		Peppino Sapia
		Valentino Pingitore
		Salvatore Lorenzo
		Tony J. G. Apollaro
		Francesco Francica
Р	PhD students	Valentina Caputi
		Diana Kenzelli Eskis Stranges
		Nadia Ligato
		Denia Marlenis Cid Perez
		Diana Carolina Coello Fiallos
		Gabriela Viaviana Tubon Usca
		Cristian Isaac Vacacela Gomez
		Michele Pisarra
	Collaborators	Raul Baragiola (Lab. for Atomic and Surface Physics, University of Virginia, Charlottesville, USA)
		W. M. Silkin (Univiersity of the Baque Country, SPAIN)
		M. J. Pitarke (Univiersity of the Baque Country, SPAIN)
		Valerio Pirronello (Din di Fisica Facoltà di Ingegneria Università di Catania Italy)
		Y.L.T. Ting (Facoltà di Scienze, Università della Calabria)
		Giulio Manicò (Dip. di Fisica, Università di Catania, Italy)
		Donatella Barca (Dip. di Scienze della Terra - UNICAL).
		Marisa Michelini (Dipartimento di Fisica, Università di Udine, Italy)
		Alberto Stefanel (Dipartimento di Fisica, Università di Udine, Italy)
		Marco Allano (Dip. Ingegneria Meccanica, Universita della Calabria) Silvia Scalese (CNR – Catania, Italy)
		Carlo Carbone (Istituto di Struttura della Materia-CNR Trieste, Italy)
		Paolo Moras (Istituto di Struttura della Materia-CNR Trieste, Italy)
		Polina Sheverdyaeva (Istituto di Struttura della Materia-CNR Trieste, Italy)
		Harald Brune (Ecole Polytechnique Fédérale de Lausanne)
		Marco Grioni ( <i>Ecole Polytechnique Fédérale de Lausanne</i> )
		YURIY Deakov (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany) Maroo Polini (CNP, Nano and Scuola Normala Superiora, Diag, Italy)
		Vittorio Pellegrini (NEST and Scuola Normale Superiore, Pisa, Italy)
		Florian Mittendorfer (Vienna University of Technology, 1040 Vienna, Austria)

M. Fonin (Universitat Konstanz, 78464 Konstanz, Germany) G. Costantini (University of Warwick, United Kingdom) Olimpia Arias de Fuentes (IMRE, La Habana, Cuba) Ernesto Pelaez (Insituto de Quimica, Universidad de la Habana, Cuba Adalgisa Tavolaro (Istituto per la Tecnologia delle Membrane (ITM) - CNR UNICAL) Leonardo Pagnotta (DIMEG UNICAL) Dennis Cazar Ramirez (Escuela Superior Politecnica de Chimborazo (ESPOCH) Riobamba, Ecuador) Zdenek Sroubek, (Czech Academy of Sciences and at the University of California-Riverside USA) John Goold (University of Oxford UK). Sabrina Maniscalco (H.W. University, Edinburgh, UK) Suzanne McEndoo (H.W. University, Edinburgh, UK) Massimo Borrelli (H.W. University, Edinburgh, UK) Pinj Haikka (H.W. University, Edinburgh, UK) Gerardo Adesso (University of Nottingham, UK) Carlos Sabin (University of Nottingham, UK) Mauro Paternostro (Queen's University, Belfast) Alessandro Cuccoli (Dipartimento di Fisica, Università di Firenze, Italy) Paola Verrucchi (ISC-CNR, Firenze, Italy) Leonardo Banchi (ISI Foundation, Torino) Ruggero Vaia (ISC-CNR, Firenze, Italy) M. G. A. Paris (Universita' di Milano), R. Zambrini (IFISC, Palma de Mallorca)

F. Galve (IFISC, Palma de Mallorca)

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 twodimensional (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.

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. Intercalation of foreign atoms into the graphene/metal interface offers an appealing possibility to control the degree of hybridization between the substrate and C- $2p_z$  orbitals.

In this respect, 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. 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.

Transition metal (TM) substrate are receiving huge and constant attention not only because of the importance of their interaction with epitaxial monolayer graphite (MG) but also for the role that transition metal oxides play in many heterogeneously catalyzed chemical reactions.

It is now quite well understood that nanometric control of few-layers oxide films on metal surfaces can allow to tune their properties as catalysts. In the group of transition metal oxides, nickel oxide is not only a prototype of an antiferromagnetic insulator with strong electron correlation, but is also of interest as main or co-catalyst in heterogeneous catalysis, or for the realization of giant magnetoresistive sensors. In heterogeneous catalysis, many reactions take place on active centers at a substrate, and the only rational approach to study such complex chemical processes is to investigate model catalysts, mainly single crystal surfaces, in ultra-high vacuum conditions.

Recently we focused on the growth of ultrathin epitaxial NiO films on Ni(111) single crystal metal substrate in order to clarify the role played by the substrate and by the film thickness. in the adsorption process.

The literature on NiO layers grown on Ni single crystals, and their reactivity towards chemical species, presents different points that have to be clarified. It is shown that even in the absence of a good matching between Ni and NiO lattice parameters, ultrathin NiO films can be quite easily grown on Ni single crystals, but it is also clear that several open questions need to be addressed by a systematic investigation, also in order to find good recipes to control thickness and atomic order. Little work has been made so far to understand the differences in oxidation kinetics, ultimate oxide thickness, morphology and chemical properties of films obtained on nickel single crystals by oxidation.

Oxide films were grown on Ni(111) substrate by exposure to background pressure of molecular oxygen at fixed temperatures. For each temperature, oxygen uptake curves were obtained by exposing the surface to different molecular oxygen pressures. For each oxidation procedure the oxygen uptake has been determined by the oxygen AES peak intensity normalized to its background in the integral mode.

The thickness of the relevant phases has been estimated by the AES peaks intensities, using a calibration procedure based on ordered oxygen phases (the p(2x2)-O phase on Ni(111)).

It has been found that on Ni(111), saturation with molecular oxygen at fixed temperatures, without subsequent annealings, gives rise to oxide layers with different features. For oxygen saturation at 300 K, OH groups seem to stabilize polar NiO(111), preventing the surface from undergoing the so-called octopolar (2x2) reconstruction.

Oxidation at 500 K gives a NiO(100) LEED, with a more regular surface almost completely covered by flat terraces. The long range order, the degree of hydroxylation, and the surface topography has been studied by LEED. Oxidation kinetics and film thicknesses were determined by AES in the 1-2 monolayers (ML) range. Electronic surface states were studied by angular-resolved EELS as a function of the oxide thickness.

All these findings once more call for a deeper investigation of the properties of ultrathin NiO layers. In this respect, it is interesting to study the growth of epitaxial monolayer graphite (MG) on the ultrathin TM oxides exploring the extent of their interaction as a function of the oxide thickness.

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

The 2012 research activity was devoted to ab-initio modeling of carbon based nanostructures, in free standing forms and deposited on metal surfaces, combined with theoretical end experimental studies of ion induced and electron induced excitations.

#### 3.2.1 Collective response of low dimensional, many body systems to an abrupt perturbation

Based on the general concept of orthogonality catastrophe in a Fermi gas, we studied the shake up properties of electrons emitted in X-ray absorption and Auger neutralization processes from carbon based nanomaterials. In particular, we considered core-hole induced electron excitations in fullerene molecules and small-diameter conducting carbon nanotubes (CNTs), using density functional theory with different basis sets plus the generalized gradient approximation for exchange and correlation. Sudden creation of the core-state was simulated by replacing a 1s electron pair, localized at a central site of the structures, with the effective pseudo-potentials of both neutral and ionized atomic carbon. Excited states were obtained from the ground state (occupied and empty) electronic structure of the ionized systems, and their overlaps with the ground state of the neutral systems were computed. Lifetime and finite-temperature corrections were applied to simulate the many-electron response of the nanoobjects. The simulated spectra of the fullerene molecule and the nanotubes were found in good agreement with x-ray photoemission experiments on thick  $C_{60}$  films and nanotube bundles, respectively. A more phenomenological approach was used describe core-valence-valence transitions from single wall CNTs, focusing on the high kinetic energy region of the spectra, where the many body shake-up of  $\pi$  electrons. The calculations were found in good agreement with available experiments. Fermi edge resonance and orthogonality catastrophe enter prominently the physics of phenomena as diverse as the Kondo effect and the scattering or sticking of a low-energy atom or ion on a metal surface. For example, recently it has been proposed to observe this universal physics in controllable ultracold atomic setups where the singular behavior may be probed either in the time domain by Ramsey interference type experiments, performed on the impurity atom, or in the frequency domain by radio-frequency spectroscopy. Our purpose is to provide such an analytic description, and discuss the transient response of a harmonically trapped Fermi gas following the sudden switching of an embedded two-level atom excited by a fast pulse.

#### 3.2.2 Electronic properties and plasmon excitations in Graphene and doped graphene

Over the recent years, the interest in graphene has impressively grown in both fundamental research and technological applications. One of the most notable examples is the raising of graphene-based electronics. To this extent, many of the peculiar properties of graphene are related to its novel electronic structure near the Fermi level, represented by the well-known Dirac cone. The realization of an acoustic plasmon, in addition to a conventional two-dimensional (2D) plasmon, is predicted to occur for carriers in the very same two-dimensional (2D) band of extrinsic (doped or gated) graphene. The origin of such a novel mode resides in the strong anisotropy that is present in the graphene band structure near the Dirac point. This fact allows for the coexistence of carriers moving with two distinct velocities along the K direction, which leads to two modes of collective oscillation: one mode in which the two types of electrons oscillate in phase with one another, and the other mode that we propose in this study corresponds to a low-frequency acoustic oscillation in which the two types of electrons oscillate out of phase. If this prediction is confirmed experimentally, it will represent the first realization of acoustic plasmons originated in the collective motion of a system of two types of carriers exited within the very same band. Although there is much debate regarding whether graphene is more suitable than metals for use in plasmonics, the useful operational frequency ranges of these materials are complementary. In addition, the damping of surface plasmons hinders the realization of nanophotonic devices. Several recent studies have uncovered some of the mid-infrared damping mechanisms for plasmons in graphene, which offer a number of unique and interesting properties.

#### 3.2.3 Abinitio simulations and spectroscopy of Graphene/Metal interfaces

The electronic structure of graphene sheets deposited on metal surfaces is still not well understood, because a detailed knowledge of the distortion of the  $\pi$  bands of free standing graphene, due to the substrate underneath is lacking. Abinitio modeling different graphene/metal interfaces, combined with experimental studies of ion induced and electron induced excitations seem to be promising for the production of large graphene areas as well as graphene based devices. We propose a systematic investigation of such materials, staring with existing density functional theory (DFT) approaches to be tested on free standing Graphene, (n,n) and (n,0) Carbon Nanotubes (CNTs), Graphene Slabs and Graphene deposited on Ni(111) substrates. We will perform both atomistic and periodic DFT computations 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, is needed to improve the ground state description of the Nickel slab.

Once the ground state properties have been determined, we will compute deep-hole excited states using ionized atomic pseudo potentials. The one-electron orbitals, entering both the ground and the excited states of the systems, will be used to calculate the energy distributions of electron ejected from the samples, via X-ray or Auger processes. Linear time-dependent DFT methods will be applied to the determination of the dielectric response of the systems, including the energy loss spectra.

The simulations will be applied to secondary electron spectroscopy experiments probing the excited states of graphene adsorbed on a Ni(111) surface. In recent studies, a fine structure directly related to the empty bands above the vacuum level of the sample was resolved in the spectra excited by electrons. Some high energy features were identified in Ion-induced spectra that are 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 curves were shown to exhibit a square root behavior, indicating the 2D character of the interface collective excitation.

#### 3.2.4 ARSEE Experiments on Graphene

Concerning the experimental side, Angle Resoved Secondary Electron Emission (ARSEE) was used to probe the excited states of grapheme adsorbed on a Ni(111) surface. ARSEE has been demonstrated in the recent past to be a powerful tool for mapping the energy dispersion of the unoccupied bands of crystalline solids. Electrons excited in empty states coupled to the vacuum are emitted conserving the surface parallel component of the momentum. This emission produces a fine structure in ARSEE spectra, which allows the absolute mapping of the dispersion of the bulk unoccupied bands of the solid sample. Observations of spectral features in SEE experiments from ultrathin graphene samples on substrates have been ascribed to the electronic properties of the overlayer and no clear signal from the bulk substrate or differences with respect to bulk graphite have been resolved. In particular the graphene-nickel(111) interface showed interesting electron emission properties that led us to focus our analysis to this system. In fact, energy distributions of electrons emitted by the Ni(111) are remarkably altered by the adsorption of graphene.

On the other hand, the total electron emission yield appears to be related to the bulk properties of the metal substrate and does not change when the graphene layer is adsorbed on the bare surface, a property that suggests graphene on metal surfaces as a protective coating in many research areas where the stability of the electron emission yields of surfaces is an important requirement, from extreme ultraviolet (EUV) litography to electron multipactor effects in particle accelerators. We performed state of the art Density Functional Theory (DFT) calculations of the electronic band structure of graphene (1 to 6 layers), graphite and graphene adsorbed on Ni(111), focusing on the unoccupied energy levels up to 50 eV above the Fermi level. The results of the calculations have been compared with observations obtained in ARSEE experiment either performed by us or reported in the literature. ARSEE measurements show spectroscopic features that can be related to energy states found in band structure calculations. The combined analysis of DFT calculations and ARSEE experiments demonstrates the role of 2D scattering resonances recently predicted in determining the secondary electron emission properties of graphene based materials.

# **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 2012, the research activity included also the study of decoherence and transport of quantum correlations in spin systems.

In particular, concerning the decoherence dynamics of open quantum systems, we have established a simple relationship between recently proposed measures of non-Markovianity and the Loschmidt echo, which holds for a purely dephasing dynamics of a quantum system coupled to a many-body environment. We showed that the Loschmidt echo is intimately related to the information flowing out from- and occasionally back into- the system. The latter, in turn, determines the non-Markovianity of the reduced dynamics of the open system. Specifically, we applied such a considerations to a central qubit coupled to a quantum Ising ring in transverse field to show how the information flux between system and environment is strongly affected by the environmental criticality: the qubit dynamics is shown to be Markovian exactly and only at the critical point. Non-Markovianity is then argued to be an indicator of criticality. We have also studied the interplay between forgetful and memory-keeping evolution enforced on a single two-level system by an N-spin environment whose elements are in turn connected to individual bosonic baths. Contrarily to the expectation that any non-Markovian effect would be buried by the forgetful mechanism induced by the spin-bath coupling, we actually showed that a full Markovian-to-non-Markovian transition of the system's dynamics takes place, controllable through the energy mismatch between the system and the spin environment.

A substantial part of our research has been devoted to study the properties of quantum correlations, in particular entanglement and quantum discord. We introduced the "discording power" of a unitary transformation, which

assesses its capability to produce quantum discord, and analyzed discord generation by relevant classes of twoqubit gates. Using the Cartan decomposition of two-qubit unitaries, and evaluating the maximum discord achievable by a unitary upon acting on classical-classical states at fixed purity, we found that there exist gates which are perfect discorders for any value of purity, and that they belong to a class of operators that includes square root of SWAP. Other gates, even those universal for quantum computation, do not possess the same property: the CNOT, for example, is a perfect discorder only for states with low or unit purity, but not for intermediate values.

We also studied the dynamics of several types of (classical and quantum) correlations in the Fermi problem. This is an archetypal model to study micro-causality in the quantum domain where two atoms, the first of which is initially excited, interact with the vacuum electromagnetic field. The process of excitation transfer towards the second atom via a flying photon generates correlations between the two atoms. In particular, we analyzed the role of the light cone in the emergence of such correlations, by investigating the dynamics of entanglement, quantum discord and classical correlations.

Furthermore, we studied the transfer of quantum correlations in spin systems. In particular, we investigated quantum information transmission in 1-D spin-1/2 systems and showed that an "almost-perfect" transfer can be achieved in the ballistic regime of an arbitrarily long chains, provided the two pairs of mirror-symmetric extremal bonds are modified.

## 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,  $\cdots$ ) form an uniform nanocomposite. The heterestructures 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  $V^0$  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.

#### 3.5.4 New materials growth for application to Graetzel photoelecrochemical cells

Single-walled carbon nanotubes (SWCNTs) or multi-walled nanotubes (MWCNTs) are produced and arranged in various context to search for their interesting and suitable properties. In particular nanocarbon structures for gas or alkali storage and photovoltaic conversion, find interesting applications in energy production at low environment impact. Open problems in this research field are numerous and range from the preparation of suitable samples (including the addition of nanostructures and/or nanoparticles for their functionality) to the understanding of the involved physical mechanisms. A parallel interesting application can be the use of nanostructures as gas sensor. In fact Carbon nanotube devices are very sensitive chemical detectors: their electrical properties (conductivity and field emission) vary strongly when they are exposed to chemicals. After the discovery of the sensitivity to NH3 (usually monitored in farms and industries) and NO<sub>2</sub> (an air pollutant from motor vehicle exhaust and other combustion sources), similar performances for many other chemical molecules, including oxygen, methane, carbon dioxide, alcohol vapour and proteins has also been reported. Carbon nanostructures (as bundles of MWCNTs and/or SWCNTs, graphene sheets) can be produced on supporting ordinary substrates or ordered crystalline structures by different methods, including: laser ablation, CVD, and. Such nanostructures are basically interesting for characterizing their properties and can be used as a component of new devices or exposed to particle fluxes (gas or vaporized alkali metals) to study their adsorption and storage capacity. At the same time the produced devices can be treated and functionalized to improve and change the above mentioned properties. Such complexes (supporting materials and nanostructures) are addressed to produce photovoltaic cells with enhanced photoelectrochemical performances, concerning the photoreponse in the visible and near-infrared regions. Recently, it has been shown that MWCNT are able to generate photocurrent with efficiency up to 7%. Novel organic solar cells have been prepared using molecular clusters of porphyrins and fullerene. These results and other studies on thermo- iono- and catodo-luminecence of nanotubes are of particular relevance for photovoltaic nanodevices and solar energy conversion applications. Further investigations demonstrate the good perspectives of nanostructures as chemical sensors, properties which can be tested through resistivity measurements at different temperatures or through the use of nanometric probes such as Atomic Force Microscopy (AFM).

The aim of this research line is to perform the fabrication of a series of samples which will be studied in view of improving their properties in relation to the above mentioned applications. The preliminary sample preparation can be characterized by testing the reproducibility, then by comparing and selecting the optimal procedures for the peculiar application. Successively the samples will be submitted to gas adsorption, alkali evaporation and/or bombardment to properly modify and control their use. In the case of photovoltaic applications the different nanostructures (SWCNTs, MWCNTs or grapheme sheets or ...) will subject to specific investigation for characterizing their performances as low-cost photovoltaic cells. In particular such studies are intended to clarify the basic role of MWCNTs in improving the IPCE (Incident Photon to current Conversion Efficiency) with respect to SWCNTs and to understand the underlying physical processes. In fact the electrical properties of alkaline metal-doped nanotubes have been characterized by resistivity measurements to elucidate the chemical effects by alkali doping. The measurements, with the same dedicated experimental apparatus, can be easily extended to the samples involving MWCNTs and will be useful to understand the electron fluxes when the same sample has been modified by the above mentioned procedures.

On the other hand, recent works demonstrate that nanotube behaviour is strongly dependent on alkaline exposure procedures (evaporation or bombardment), such behaviours are interesting for designing efficient sensors and electronic devices. The adhesion of gas molecules on the surface of a nanotube, which can be investigated by STM techniques, could create a nano-protrusion which reduces the work function and strongly influences the field emission properties of the tube. We will focus on experimental methods to determine the effect and the sensing mechanism of different chemicals.

## 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 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 in the energy inter-conversion among different forms: in this connection, a class of analogous systems (the "two-capacitor-like" systems) has been thoroughly investigated in a comparative way.

#### A. PUBLICATIONS

## A.1 Publications on international journals

- A.1.1 Publications on international journals printed in 2012
  - P. Barone, M. Barberio, A. Bonanno, A. Oliva, *A new purification technique for single-walled carbon nanotubes by interaction with alkali and oxygen*, Journal of Nanoscience and Nanotechnolgy, 12, 5039 (2012)
  - M. Barberio, P. Barone, V. Pingitore and A. Bonanno, *Optical properties of TiO2 anatase – Carbon Nanotubes composites studied by cathodoluminescence spectroscopy*, Superlattice and Microstructure 51, 177 (2012)
  - M. Barberio, P. Barone, R. Vasta, G. Manicò and F. Xu, Formation of Nitrogen and diazene by electron irradiation of solid ammonia, Thin Solid Films, 520, 5479 (2012)
  - M. Barberio, P. Barone and A. Oliva, *Optical and morphological properties of ZnS – Carbon Nanotubes composites studied by cathodoluminescence spectroscopy*, Radiation Chemistry and Physics, 81, 642 (2012)
  - P. Barone, M. Barberio, A. Oliva and A. Bonanno, Synthesis and characterization of carbon nanotubes wrapped on anatase microparticles, Particle & Particle Systems Characterization, 28, 64 (2012)
  - M. Giarola, G. Mariotto, M. Barberio, D. Ajò, *Raman spectroscopy in gemology as seen from a jeweller's point of view*, Journal of Raman Spectroscopy DOI 10.1002/jrs.4129 (2012)
  - M. Barberio, P. Barone V. Pingitore, A. Bonanno, UV luminescence emission from LiF – Carbon Nanotubes composites, Superlattice and Microstructures, 52, 1053 (2012)
  - M. Barberio, P. Barone, A. Imbrogno, V. Pingitore, F. Xu, A. Bonanno, *Optical and structural properties of carbon nanotube–rutile heterostructures*, Journal of Chemistry and Chemical Engineering USA 6 199-208 (2012)
  - V. Pingitore, M. Barberio, P. Barone, A. Oliva, *Photoluminescence emission from Carbon Notubes based composites*, Nanoscience and Nanotechnology Letters, 4, 1082-1086 (2012)
  - P. Barone, M. Barberio, V. Pingitore and A. Bonanno, *Transport properties of alkali-doped multi walled carbon nanotubes*, Journal of Nanoscience and Nanotechnology, 12 9295-9298 (2012)
  - A. Bonanno, M. Camarca and P. Sapia, Reaching equilibrium: the role of dissipation in analogous systems, within a thermodynamic-like perspective, European Journal of Physics 33 (2012) 1851–1869
  - D. Topwal, U. Manju, D. Pacilè, M. Papagno, D. Wortmann, G. Bihlmayer, S. Blugel, and C. Carbone, *Quantum electron confinement in closely matched metals: Au films on Ag(111)*, Phy. Rev. B 86, 085419 (2012).
  - 13. M. Papagno, D. Pacilè, D. Topwal, P. Moras, P. M. Sheverdyaeva, F. D. Nattarer, A. Lehnert, S. Rusponi, Q. Dubout, F. Calleja, E. Frantzeskakis, S. Pons, J. Fujii, I. Vobornik, M. Grioni, C. Carbone, and H. Brune,

*Two distinct phases of bilayer graphene films on Ru(0001)*, ACSNano **6**, 9299 (2012).

- M. Papagno, S. Rusponi, P. M. Sheverdyaeva, S. Vlaic, M. Etzkorn, D. Pacilé, P. Moras, C. Carbone, and H. Brune, *Large band gap opening between graphene Dirac cones induces by Na adsorption onto an Ir superlattice*, ACSNano 6, 199 (2012).
- Y. Wang, S. Fabris, T. W. White, F. Pagliuca, P. Moras, D. Topwal, P. M. Sheverdyaeva, C. Carbone, M. Lingenfelder, T. Classen, K. Kern, G. Costantini, Varying molecular interactions by coverage in supramolecular surface chemistry, Chem. Commun. 48, 534-536 (2012).
- F. D. Natterer, S. Rusponi, M. Papagno, C. Carbone, H. Brune, *Optimizing long-range order, band gap, and group velocities for graphene on close-packed metal surfaces,* J. of Phys. Cond. Matter 24, 314203 (2012).
- A. Cupolillo N. Ligato, L. S. Caputi, *Two-dimensional character of the interface-p plasmon in epitaxial graphene on Ni(111)*. CARBON, vol. 50, p. 2588-2591 (2012)
- P. Riccardi, A. Cupolillo, M. Pisarra, A. Sindona, L S Caputi Primary energy dependence of secondary electron emission from graphene adsorbed on Ni(111). APPLIED PHYSICS LETTERS, vol. 101, 183102 (2012)
- M. Pisarra, P. Riccardi, A. Cupolillo, A. Sindona, L S Caputi Studies of electron emission in the interaction of electrons with graphene on Ni(111) Surface. NANOSCIENCE AND NANOTECHNOLOGY LETTERS, vol. 4, 1465 (2012)
- A. Sindona, M. Pisarra, P. Riccardi, G. Falcone Cluster and Periodic Density Functional Study of Auger Electron Emission from Conducting Carbon Nanotubes NANOSCIENCE AND NANOTECHNOLOGY LETTERS 4, 1462, (2012)
- P. Haikka, J. Goold, S. McEndoo, F. Plastina and S. Maniscalco, *Non-markovianity, Loschmidt echo, and criticality: A unified picture* Phys. Rev. A 85, 060101(R) (2012). Also selected by Virtual Journal of Quantum Information, Vol. 12, Issue 6, 2012.
- T.J.G. Apollaro, L. Banchi, A. Cuccoli, R. Vaia, and P. Verrucchi, 99%-fidelity ballistic quantum-state transfer through long uniform channels Phys. Rev. A 85, 052319 (2012).
- M. Borrelli, C. Sabin, G. Adesso, F. Plastina, S. Maniscalco, Dynamics of atom-atom correlations in the Fermi problem New J. Phys. 14, 103010 (2012).

#### A.1.2 Publications on international journals accepted in 2012

- M. Barberio, V. Pingitore, P. Barone, M. Davoli, F. Stranges, F. Xu, A. Bonanno, Synthesis of carbon nanotube/TiO2 composites by titanium evaporation in ultra high vacuum ambient, Microelectronics Engineering in press, DOI: http://dx.doi.org/10.1016/j.mee.2012.12.016 (2013)
- M. Barberio, R. Vasta, P. Barone, G. Manicò, F. Xu, Experimental and theoretical study on the ethane and acetylene formation from electron irradiation of methane ices, World Journal of Condensed Matter Physics (in press – accepted october 2012)

- 3. A. Bonanno, M. Camarca, P. Sapia, *The Casimir effect: A multimedia and hands-on integrated approach*, International Journal on Hands-on Science. In press, 2013
- D. Pacilè, P. Leicht, M. Papagno, P. M. Sheverdyaeva, P. Moras, C. Carbone, K. Krausert, L. Zielke, M. Fonin, Y. S. Dedkov, F. Mittendorfer, J. Doppler, A. Garhofer, and J. Redinger, Phy. Rev. B 87, 035420 (2013).
- Cupolillo A, Ligato N, Caputi L S. Low Energy Two-dimensional Plasmon in Epitaxial Graphene on Ni(111). Surface Science in press, DOI: 10.1016/j.susc.2012.09.018
- Ligato N, Cupolillo A, Caputi L.S. *Study of the intercalation of graphene on Ni(111) with Cs atoms: Towards the quasi-free graphene* Thin Solid Films in press DOI: 10.1016/j.tsf.2013.02.121
- A. Sindona, M. Pisarra, F. Naccarato, P. Riccardi, F. Plastina, A. Cupolillo, N. Ligato, L. S. Caputi, G. Falcone, *Core hole effects in fullerene molecules and small-diameter conducting nanotubes: a density functional theory Study* J. Phys.: Condens. Matter 25, 115301 (2013). DOI: 10.1088/0953-8984/25/11/115301
- T. J. G. Apollaro, S. Lorenzo, F. Plastina, *Transport of Quantum Correlations across a spin chain*, Int. J. of Mod. Phys. B 27, 1345035 (2013).
- F. Galve, F. Plastina, M. G. A. Paris, and R. Zambrini, Discording power of quantum evolutions, Phys. Rev. Lett. 110, 010501 (2013).
- S. Lorenzo, F. Plastina, M. Paternostro, *Tuning non-Markovianity by spin-dynamics control* Phys. Rev. A 87, 022317 (2013).

#### A.1.3 Papers submitted for publication in 2012

- M. Barberio, P. Barone, F. Xu, A. Bonanno, Silver nanoparticles synthesized by laser ablation in acetone: influence of ablation time and their reactivity with oxygen in the air, Physica E, (submitted, October 2012)
- M. Barberio, P. Barone, V. Pingitore, F. Xu, *Photoluminescence from Silver/Carbon Nanotubes Composites, Superlattice and Microstructures* (submitted december 2012)
- A. Cupolillo, N. Ligato, L.S. Caputi. *Plasmon dispersion in quasi-freestanding graphene on Ni(111)*. Submitted to Applied Physics Letters

## **B PUBLICATIONS ON CONFERENCE PROCEEDINGS**

## **B.1** Publications on international conference proceedings in 2012

- A. Bonanno, G. Bozzo, M. Camarca, M. Michelini, P. Sapia, *Free Ideas: Results from an innovative project for teacher development in Calabria (Italy),* Proceedings of the "International Research Group on Physics Teaching" 2011 Conference (GIREP 2011). University of Jyväskylä, Finland, 1 - 5 August 2011.
- N. Ligato, A. Cupolillo, L.S. Caputi, *Intraband plasmon dispersion in graphene/Ni(111)* 4th International Conference on Nano-Structures Self-Assembly (NanoSEA 2012) 25-29 June 2102 Sardinia (Italy)

## **B.2** Publications on international conference proceedings in 2012

 M. Alfano, S. Pini, M. Barberio, G. Chiodo, A. Pirondi, F. Furgiuele, Surface patterning of metal substrates INDUCED by laser ablation for improved adhesive bonding, Atti del convegno AIAS 2012

## C BOOK CHAPTERS

 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 (2012). ISBN 978-88-548-4935-8

## D INVITED PRESENTATIONS

#### D.1 Invited presentations at international conferences in 2012

- M. Papagno, *Tailoring the Electronic Properties of Epitaxial Graphene on Metallic Substrates*, 4rd International Conference Smart Materials Structures Systems 4-10 June 2012, Montecatini Terme-Italy
- F. Plastina, Decoherence, non-Markovianity and orthogonality catastrophe, Quantum twin workshop 2012, Favignana (TP) 02-06-2012.
- T. J. G. Apollaro, *High-quality quantum-state transfer through long uniform channels*, IQIS2012, Padova 26-28 settembre 2012

#### D.2 Invited presentations at national conferences in 2012

 D. Pacilé, *A novel mismatched graphene-Ni(111) surface*, Società Italiana di Fisica 2012 (September 17-21, Napoli)

## **E PRESENTATIONS AT CONFERENCES**

## E.1 Oral Presentations at international conferences in 2012

 N. Ligato, *Intraband plasmon dispersion in graphene/Ni(111)* 4th International Conference on Nano-Structures Self-Assembly (NanoSEA 2012) 25-29 June 2102 Cagliari (Italy)

## 2. A. Sindona,

Dielctric properties of graphene/metal interfaces, 4th International Conference on Nano-Structures Self-Assembly (NanoSEA 2012) 25-29 June 2102 Cagliari (Italy)

3. A. Sindona,

Many electron shake up in fulerenes and nanotubes, NANOSCIENCE AND NANOTECHNOLOGY 01-04 October 2012, FRASCATI, ROME (ITALY)

- M. Pisarra, Loss function of graphene and doped graphene, NANOSCIENCE AND NANOTECHNOLOGY 01-04 October 2012, FRASCATI, ROME (ITALY)
- 5. F. Plastina,

Loschmidt echo, non-Markovianity and orthogonality catastrophe, 44-th symposium on Mathematical Physics, "New Developments in the Theory of Open Quantum Systems", Torun (Polonia) 22-06-2012.

6. F. Plastina,

Loschmidt echo, non-Markovianity and orthogonality catastrophe, Capri Fall Workshop on "Non equilibrium processes & fluctuation-dissipation theorems", Anacapri (NA) 13-09-2012

## E.2 Presentations at national conferences in 2012

M. Papagno,

*Tailoring the electronic properties of epitaxial graphene on metallic substrates*, SILS 2012 (July 18-20, Rende, Italy)

## 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
1 051400 jenows	D. Salvatore
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:

30. 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).

31. Study of proton-proton interactions with the ATLAS experiment at the LHC accelerator of the CERN Laboratory (Geneva, Switzerland).

32. Study of a forward physics detector for ATLAS experiment (AFP) and for medical applications.

33. R&D of hadronic calorimeter modules based on the Dual Readout Method (DREAM).

34. Study of the electron-positron interactions at the centre of mass energy 1020 MeV with KLOE apparatus at DAFNE collider of LNF Laboratory (Rome, Italy).

35. 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. MastroberardinoM. SchioppaG. SusinnoE. 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 30 GeV and 920 GeV 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  $\sim 320$ GeV, much larger than previously achieved in such collisions, and allowing to probe the proton structure down to distance scales as low as  $10^{-18}$ 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  $10^5$  GeV<sup>2</sup>/c<sup>2</sup>) 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 2012 year we have continued to contribute to:

17. the combination of the ZEUS and H1 inclusive results and determination of the proton parton distribution functions;

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

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

#### International collaboration

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,  $M_t=170$  GeV/c<sup>2</sup>. 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).

On 4 July 2012 the ATLAS and CMS Collaborations jointly announced the independent discovery of a previously unknown neutral boson, compatible with the Higgs Boson, with a mass in the range 125-127 GeV/ $c^2$ . Fig. 2 shows a representative result drawn from the latest ATLAS publication (Phys. Lett. B716 (2012) 1-29) that, using an increased data sample and improved analysis techniques, has increased the the discovery significance to 5.9-sigma (1 in 588 million chance of being due to random background effects) and measured a mass value of  $126.0 \pm 0.4$  (stat)  $\pm 0.4$  (sys) GeV/ $c^2$ . The new particle appears to be fully compatible with the production and decay properties of the Standard Model Higgs Boson.



Fig. 2 The local probability  $p_0$  for a background-only experiment to be more signal-like than the observation as a function of  $m_H$  reported in Phys. Lett. B 716 (2012) 1-29. The dashed curve shows the median expected local  $p_0$  under the hypothesis of a Standard Model Higgs boson production signal at that mass. The horizontal dashed lines indicate the p-values corresponding to significances of  $1\sigma$  to  $6\sigma$ .

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):

- 4. 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;
- 5. 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;
- 6. 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 2012 the Unical HEP group gave a major contribution to the following ATLAS activities:

- 13. 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.
- 14. Development and maintenance of the Gnam package, the low-level data acquisition software for the ATLAS subdetector 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 subdetectors 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.
- 15. 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.

- 16. 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.
- 17. 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 the 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 and top quark 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 year 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. 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. In the field of top production we are contributing to the measurement of the single differential cross sections for top pairs production in the semileptonic channels, where events in the electron/muon plus jets channel are isolated, using the 2001 and 2012 data samples.
- Study of the Long-Lived particles of the Hidden Valley sector. Several extensions of the SM predict the existence 18. 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 v-pion ( $\pi_{\rm V}$ ), 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-1 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. Another analysis started as an extension of the previous one. The aim is to explore the lepton jet production at 8 GeV centre of mass energy, not only muons, and with the whole statistics collected during the 2012 data taking. Another analysis exploits the  $\pi_{\rm V}$  decays in the ATLAS hadronic calorimeter: in this scenario, the long-lived particles deposit most of their energy in there and very little or none in the electromagnetic calorimeter, and also have few or no charged tracks pointing at the hadronic energy deposits. A signature-driven trigger that optimizes the acceptance for this class of event is used to select events at the trigger level. Background processes, dominated by Cosmic contamination and QCD dijet production, require special attention: these backgrounds are further suppressed in this analysis by requiring both  $\pi_V$  to decay in the calorimeter. The analysis was started on the 5 fb<sup>-1</sup> collected at 7 TeV in 2011 and it is mostly completed for the 2012 20.8 fb<sup>-1</sup> at 8 TeV. Limits on the cross section for this kind of signal are set as a function of the long-lived particle lifetime.

#### 4.3 HADRONIC CALORIMETRY

Physicists:	<u>L. La Rotonda</u>
-	A. Policicchio
	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.

To these project, an Italian collaboration (Bologna, Cagliari, Cosenza, Roma1, Pavia) together with U.S. Researchers is working since 2006. MIUR has considered this project as a PRIN (Progetto di Ricerca di Interesse Nazionale) and has funded it in the period 2010-2012. In the summer of 2011 the same project has also been accepted as an official CERN R&D experiment.

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.

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 (PbWO4) 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. 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 2012 a new fiber calorimeter has been produced and tested. It consisted of 9 lead-based modules and 2 copper based modules. Each module contains 4 towers and is read out by 8 PMTs, 4 for the Cerenkov channels and 4 for the scintillation channels. Each module is 2.5 m long (10  $\lambda_{int}$ ), has a cross section of 9.2 x 9.2 cm<sup>2</sup> and a fiducial mass of about 150 Kg. Each tower contains 1024 plastic optical fibers (diameter 1.0 mm, equal numbers of scintillating and clear fibers). Each tower produces two signals, a scintillation signal and a Cerenkov signal which are

detected by separated PMts. This calorimeter has been tested in November/December 2012.

Obtained results show a better energy resolution and linearity respect to the original DREAM calorimeter. Analyses are going on.

The Cosenza researchers participated 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  $e^+e^-$  > gamma\* -> PHI. This meson is made of strange – anti-strange quarks; has 1020 MeV/c2 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-1 (2001-2006) the collider has produced 10^10 PHI-mesons and than about 10^10 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 superconductive 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-1) 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 2012

- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of isolated diphoton cross-section in pp collision at √s = 7 TeV with the ATLAS detector*. Phys. Rev. D85 (2012) 012003
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Measurement of the top quark pair production cross section in pp collisions at √s = 7 TeV in dilepton final states with ATLAS. Phys. Lett. B707 (2012) 459-477
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of the W to tau nu Cross Section in pp Collisions at √s = 7 TeV with the ATLAS experiment.* Phys. Lett. B706 (2012) 276-294
- 4. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. A measurement of the ratio of the W and Z cross sections with exactly one associated jet in pp collisions at √s = 7 TeV with ATLAS. Phys. Lett. B708 (2012) 221-240
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for a heavy Standard Model Higgs boson in the channel H->ZZ->llqq using the ATLAS detector. Phys. Lett. B707 (2012) 27-45
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Performance of missing transverse momentum reconstruction in proton-proton collisions at 7 TeV with ATLAS*. Eur. Phys. J. C72 (2012) 1844
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of the centrality dependence of the charged particle pseudorapidity distribution in lead-lead collisions at* √s<sub>NN</sub> = 2.76 TeV with the ATLAS detector. Phys. Lett. B710 (2012) 363-382
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of the pseudorapidity and transverse momentum dependence of the elliptic flow of charged particles in lead-lead collisions at* √s<sub>NN</sub> = 2.76 TeV with the ATLAS detector. Phys. Lett. B707 (2012) 330-348
- 9. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of the transverse momentum distribution of W bosons in pp collisions at √s = 7 TeV with the ATLAS detector*. Phys. Rev. D85 (2012) 012005
- 10. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for New Physics in the Dijet Mass Distribution using 1 fb<sup>-1</sup> of pp Collision Data at √s = 7 TeV collected by the ATLAS Detector.
  Phys. Lett. B 708 (2012) 37-54
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Measurements of the electron and muon inclusive cross-sections in proton-proton collisions at √s = 7 TeV with the ATLAS detector. Phys. Lett. B707 (2012) 438-458
- 12. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.

*Measurement of the cross-section for b-jets produced in association with a Z boson at*  $\sqrt{s} = 7$  *TeV with the ATLAS detector.* Phys. Lett. B706 (2012) 295-313

- 13. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of the cross section for the production of a W boson in association with b-jets in pp collisions at √s = 7 TeV with the ATLAS detector*. Phys. Lett. B707 (2012) 418-437
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for displaced vertices arising from decays of new heavy particles in 7 TeV pp collisions at ATLAS. Phys. Lett. B707 (2012) 478-496
- 15. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for New Phenomena in ttbar Events With Large Missing Transverse Momentum in Proton-Proton Collisions at √s = 7 TeV with the ATLAS Detector. Phys. Rev. Lett. 108 (2012) 041805
- 16. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of the inclusive W+- and Z/gamma cross sections in the electron and muon decay channels in pp collisions at √s = 7 TeV with the ATLAS detector*. Phys. Rev. D85 (2012) 072004
- 17. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for supersymmetry in final states with jets, missing transverse momentum and one isolated lepton in √s = 7 TeV pp collisions using 1 fb<sup>-1</sup> of ATLAS data. Phys. Rev. D85 (2012) 012006
- 18. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for squarks and gluinos using final states with jets and missing transverse momentum with the ATLAS detector in √s = 7 TeV proton-proton collisions. Phys. Lett. B710 (2012) 67-85
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Performance of the ATLAS Trigger System in 2010*. Eur. Phys. J. C72 (2012) 1849
- 20. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Electron performance measurements with the ATLAS detector using the 2010 LHC proton-proton collision data. Eur. Phys. J. C72 (2012) 1909
- 21. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Measurement of the ZZ production cross section and limits on anomalous neutral triple gauge couplings in proton-proton collisions at √s = 7 TeV with the ATLAS detector. Phys. Rev. Lett. 108 (2012) 041804
- 22. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. A measurement of the material in the ATLAS inner detector using secondary hadronic interactions. JINST 7 (2012) P01013
- 23. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Searches for supersymmetry with the ATLAS detector using final states with two leptons and missing transverse momentum in √s = 7 TeV proton-proton collisions. Phys. Lett. B709 (2012) 137-157
- 24. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for strong gravity signatures in same-sign dimuon final states using the ATLAS detector at the LHC. Phys. Lett. B709 (2012) 322-340

- 25. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Kshort and Lambda production in pp interactions at*  $\sqrt{s} = 0.9$  and 7 TeV measured with the ATLAS detector at the LHC. Phys. Rev. D85 (2012) 012001
- 26. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of the production cross section for Z/gamma\* in association with jets in pp collisions at √s = 7 TeV with the ATLAS Detector*. Phys. Rev. D85 (2012) 032009
- 27. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for Diphoton Events with Large Missing Transverse Energy with 1 fb<sup>-1</sup> of 7 TeV Proton-Proton Collision Data with the ATLAS Detector. Phys. Lett. B710 (2012) 519-537
- 28. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Measurement of the WZ production cross section and limits on anomalous triple gauge couplings in proton-proton collisions at √s = 7 TeV with the ATLAS detector. Phys. Lett. B709 (2012) 341-357
- 29. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for extra dimensions using diphoton events in 7 TeV proton-proton collisions with the ATLAS detector. Phys.Lett. B710 (2012) 538-556
- 30. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for the Higgs boson in the H -> WW(\*) -> l nu l nu decay channel in pp collisions at √s = 7 TeV with the ATLAS detector.
  Phys. Rev. Lett. 108, 111802 (2012)
- 31. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for Production of Resonant States in the Photon-Jet Mass Distribution using pp Collisions at √s = 7 TeV collected by the ATLAS Detector.
  Phys. Rev. Lett. 108, 211802 (2012)
- 32. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for scalar bottom pair production with the ATLAS detector in pp collisions at  $\sqrt{s} = 7$  TeV. Phys. Rev. Lett. 108, 181802 (2012)
- 33. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of D\*+/- meson production in jets from pp collisions at*  $\sqrt{s} = 7$  *TeV with the ATLAS detector*. Phys. Rev. D85 (2012) 052005
- 34. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for first generation scalar leptoquarks in pp collisions at  $\sqrt{s} = 7$  TeV with the ATLAS detector. Phys. Lett. B709 (2012) 158-176
- 35. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Observation of a new chi\_b state in radiative transitions to Upsilon(1S) and Upsilon(2S) at ATLAS. Phys. Rev. Lett. 108 (2012) 152001
- Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.

Search for heavy vector-like quarks coupling to light generations in proton-proton collisions at  $\sqrt{s} = 7$  TeV with the *ATLAS detector*. Phys. Lett. B712 (2012) 22-39

- 37. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. *Measurement of inclusive jet and dijet production in pp collisions at* √s = 7 *TeV using the ATLAS detector*.
  Phys. Rev. D86 (2012) 014022
- 38. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C. Search for anomalous production of prompt like-sign muon pairs and constraints on physics beyond the Standard Model with the ATLAS detector. Phys. Rev. D 85, 032004 (2012)
- 39. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Study of jets produced in association with a W boson in pp collisions at  $\sqrt{s} = 7$  TeV with the ATLAS detector. Phys. Rev. D85 (2012) 092002
- 40. 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 the single lepton channel. Phys. Lett. B711 (2012) 244-263
- 41. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Rapidity gap cross sections measured with the ATLAS detector in pp collisions at  $\sqrt{s} = 7$  TeV. Eur. Phys. J. C72 (2012) 1926
- 42. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Search for excited leptons in proton-proton collisions at  $\sqrt{s} = 7$  TeV with the ATLAS detector. Phys. Rev. D85 (2012) 072003
- 43. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for Contact Interactions in Dilepton Events from pp Collisions at  $\sqrt{s} = 7$  TeV with the ATLAS Detector. Phys. Lett. B712 (2012) 40-58
- 44. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for decays of stopped, long-lived particles from 7 TeV pp collisions with the ATLAS detector.
  Eur. Phys. J. C72 (2012) 1965
- 45. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. *Combined search for the Standard Model Higgs boson using up to 4.9 fb<sup>-1</sup> of pp collision data at √s = 7 TeV with the ATLAS detector at the LHC.*Phys. Lett. B710 (2012) 49-66
- 46. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for the Standard Model Higgs boson in the decay channel H->ZZ(\*)->4l with 4.8 fb<sup>-1</sup> of pp collisions at √s =7 TeV with ATLAS.
  Phys. Lett. B710 (2012) 383-402

- 47. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for the Standard Model Higgs boson in the diphoton decay channel with 4.9 fb<sup>-1</sup> of pp collisions at √s =7 TeV with ATLAS.
  Phys. Rev. Lett. 108, 111803 (2012)
- 48. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Search for Pair Production of a Heavy Up-Type Quark Decaying to a W Boson and a b Quark in the Lepton+Jets Channel with the ATLAS Detector. Phys. Rev. Lett. 108 (2012) 261802
- 49. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Search for pair-produced heavy quarks decaying to Wq in the two-lepton channel at ATLAS at  $\sqrt{s} = 7$  TeV. Phys. Rev. D86 (2012) 012007
- 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 cross section for top-quark pair production in pp collisions at √s = 7 TeV with the ATLAS detector using final states with two high-pT leptons.
  JHEP 1205 (2012) 059
- 51. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Search for anomaly-mediated supersymmetry breaking with the ATLAS detector based on a disappearing-track signature in pp collisions at  $\sqrt{s} = 7$  TeV. Eur. Phys. J. C72 (2012) 1993
- 52. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Search for same-sign top quark production and fourth-generation down-type quarks in pp collisions at  $\sqrt{s} = 7$  TeV with the ATLAS detector. JHEP 1204 (2012) 069
- 53. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Search for down-type fourth generation quarks with the ATLAS Detector in events with one lepton and hadronically decaying W bosons. Phys. Rev. Lett. 109 (2012) 032001
- 54. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for FCNC single top-quark production at √s =7 TeV with the ATLAS detector. Phys. Lett. B712 (2012) 351-369
- 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 azimuthal ordering of charged hadrons with the ATLAS detector. Phys. Rev. D86 (2012) 052005
- 56. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for new particles decaying to ZZ using final states with leptons and jets with the ATLAS detector in √s = 7 TeV proton-proton collisions.
  Physics Letters B 712 (2012) 331-350

- 57. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for a light Higgs boson decaying to long-lived weakly-interacting particles in proton-proton collisions at √s = 7 TeV with the ATLAS detector.
  Phys. Rev. Lett. 108 (2012) 251801
- Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Single hadron response measurement and calorimeter jet energy scale uncertainty with the ATLAS detector at the LHC. Eur. Phys. J. C73 (2013) 2305
- 59. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.
  Measurement of the polarisation of W bosons produced at large momentum transfer in pp collisions at √s = 7 TeV with the ATLAS experiment at the LHC.
  Eur. Phys. J. C72 (2012) 2001
- 60. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C.
  Search for second generation scalar leptoquarks in pp collisions at √s = 7 TeV with the ATLAS detector. Eur. Phys. J. C72 (2012) 2151
- 61. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C. Forward-backward correlations and charged-particle azimuthal distributions in pp interactions using the ATLAS detector. JHEP 1207 (2012) 019
- 62. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurement of the production cross section of an isolated photon associated with jets in proton-proton collisions at √s* = 7 *TeV with the ATLAS detector*.
  Phys. Rev. D 85, 092014 (2012)
- 63. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Measurement of the azimuthal anisotropy for charged particle production in √s<sub>NN</sub> = 2.76 TeV lead-lead collisions with the ATLAS detector.
  Phys. Rev. C86 (2012) 014907
- 64. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Measurement of inclusive two-particle angular correlations in pp collisions with the ATLAS detector at the LHC. JHEP 1205 (2012) 157
- 65. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Determination of the strange quark density of the proton from ATLAS data on W-> lnu and Z->ll cross-sections. Phys. Rev. Lett. 109 (2012) 012001
- 66. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurement of the charge asymmetry in top quark pair production in pp collisions at √s = 7 TeV using the ATLAS detector.*Eur. Phys. J. C72 (2012) 2039
- 67. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C

*Observation of spin correlation in tibar events from pp collisions at*  $\sqrt{s} = 7$  *TeV using the ATLAS detector.* Phys. Rev. Lett. 108, 212001 (2012)

- 68. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Jet mass and substructure of inclusive jets in √s = 7 TeV pp collisions with the ATLAS experiment.* JHEP 1205 (2012) 128
- 69. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurement of ttbar production with a veto on additional central jet activity in pp collisions at √s = 7 TeV using the ATLAS detector*.
  Eur. Phys. J. C72 (2012) 2043
- 70. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for heavy neutrinos and right-handed W bosons in events with two leptons and jets in pp collisions at  $\sqrt{s} = 7$  TeV with the ATLAS detector. Eur. Phys. J. C72 (2012) 2056
- 71. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for gluinos in events with two same-sign leptons, jets and missing transverse momentum with the ATLAS detector in pp collisions at √s = 7 TeV.
  Phys. Rev. Lett. 108, 241802 (2012)
- 72. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Measurement of the Top Quark Mass with the Template Method in the ttbar -> lepton+jets Channel using ATLAS Data. Eur. Phys. J. C72 (2012) 2046
- 73. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurement of the WW cross section in √s = 7 TeV pp collisions at ATLAS and limits on anomalous gauge couplings.* Phys. Lett. B 712 (2012) 289-308
- 74. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for supersymmetry in pp collisions at  $\sqrt{s} = 7$  TeV in final states with missing transverse momentum and b-jets with the ATLAS detector. Phys. Rev. D 85, 112006 (2012)
- 75. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for Events with Large Missing Transverse Momentum, Jets, and at Least Two Tau Leptons in 7 TeV Proton-Proton Collision Data with the ATLAS Detector. Phys. Lett. B 714 (2012) 180-196
- 76. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for the decay B^0\_s->mu+mu- with the ATLAS detector. Phys. Lett. B 713 (2012) 387-407
- 77. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for pair production of a new quark that decays to a Z boson and a bottom quark with the ATLAS detector. Phys. Rev. Lett. 109 (2012) 071801

- 78. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for resonant WZ production in the WZ to Inul'l' channel in  $\sqrt{s} = 7$  TeV pp collisions with the ATLAS detector. Phys. Rev. D85 (2012) 112012
- 79. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for charged Higgs bosons decaying via H+ -> tau+nu in ttbar events using 4.6 fb<sup>-1</sup> of pp collision data at √s = 7 TeV with the ATLAS detector.
  JHEP 1206 (2012) 039
- 80. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for supersymmetry with jets, missing transverse momentum and at least one hadronically decaying tau lepton in proton-proton collisions at √s = 7 TeV with the ATLAS detector.
  Phys. Lett. B 714 (2012) 197-214
- 81. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for TeV-scale Gravity Signatures in Final States with Leptons and Jets with the ATLAS Detector at √s = 7 TeV. Phys. Lett. B 716 (2012) 122-141
- 82. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for supersymmetry in events with three leptons and missing transverse momentum in √s = 7 TeV pp collisions with the ATLAS detector.
  Phys. Rev. Lett. 108 (2012) 261804
- 83. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurement of tau polarization in W->tau nu decays with the ATLAS detector in pp collisions at √s = 7 TeV.* Eur. Phys. J. C72 (2012) 2062
- 84. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for Scalar Top Quark Pair Production in Natural Gauge Mediated Supersymmetry Models with the ATLAS Detector in pp Collisions at √s = 7 TeV.
  Phys. Lett. B 715 (2012) 44-60
- 85. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for Lepton Flavour Violation in the emu Continuum with the ATLAS detector in √s = 7 TeV pp collisions at the LHC.
  Eur. Phys. J. C72 (2012) 2040
- 86. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for a fermiophobic Higgs boson in the diphoton decay channel with the ATLAS detector. Eur. Phys. J. C72 (2012) 2157
- 87. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for tb resonances in proton-proton collisions at √s = 7 TeV with the ATLAS detector. Phys. Rev. Lett. 109 (2012) 081801
- Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C

Measurement of the top quark pair cross section with ATLAS in pp collisions at  $\sqrt{s} = 7$  TeV using final states with an electron or a muon and a hadronically decaying tau lepton. Phys. Lett. B 717 (2012) 89-108

- 89. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurement of W gamma and Z gamma production cross sections in pp collisions at*  $\sqrt{s} = 7$  *TeV and limits on anomalous triple gauge couplings with the ATLAS detector.* Phys. Lett. B 717 (2012) 49-69
- 90. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Measurement of W boson polarization in top quark decays with the ATLAS detector. JHEP 1206 (2012) 088
- 91. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurement of the t-channel single top-quark production cross section in pp collisions at* √s = 7 *TeV with the ATLAS detector*.
  Phys. Lett. B 717 (2012) 330-350
- 92. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *A search for ttbar resonances with the ATLAS detector in 2.05 fb<sup>-1</sup> of proton-proton collisions at √s = 7 TeV*. Eur. Phys. J. C72 (2012) 2083
- 93. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Evidence for the associated production of a W boson and a top quark in ATLAS at*  $\sqrt{s} = 7$  *TeV*. Phys. Lett. B 716 (2012) 142-159
- 94. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for a Standard Model Higgs boson in the H -> ZZ -> llnunu decay channel using 4.7 fb<sup>-1</sup> of √s = 7 TeV data with the ATLAS detector.
  Phys. Lett. B 717 (2012) 29-48
- 95. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *A search for flavour changing neutral currents in top-quark decays in pp collision data collected with the ATLAS detector at √s = 7 TeV.*JHEP 09 (2012)139
- 96. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for the Standard Model Higgs boson in the H -> WW -> lvlv decay mode with 4.7 fb<sup>-1</sup> of ATLAS data at √s = 7 TeV.
  Phys. Lett. B 716 (2012) 62-81
- 97. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Hunt for new phenomena using large jet multiplicities and missing transverse momentum with ATLAS in 4.7fb<sup>-1</sup> of √s = 7 TeV proton-proton collisions.
  JHEP 1207 (2012) 167
- 98. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Measurement of event shapes at large momentum transfer with the ATLAS detector in pp collisions at  $\sqrt{s} = 7$  TeV.
Eur. Phys. J. C72 (2012) 2211

99. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
Measurement of the b-hadron production cross section using decays to D\*muX final states in pp collisions at √s = 7 TeV with the ATLAS detector.
Nucl. Phys. B 864 (2012) 341-381

- 100. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for a Standard Model Higgs in the mass range 200-600 GeV in the channel H -> ZZ -> llqq with with the ATLAS detector.
  Phys. Lett. B 717 (2012) 70-88
- 101. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C ATLAS measurements of the properties of jets for boosted particle searches. Phys. Rev. D 86 (2012) 072006
- 102. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for the Higgs boson in the H->WW->Inujj decay channel at √s = 7 TeV with the ATLAS detector. Phys. Lett. B 718 (2012) 391- 410
- 103. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for the Standard Model Higgs boson in the H to tau+ tau- decay mode in √s = 7 TeV pp collisions with ATLAS. JHEP 09 (2012) 070
- 104. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for the Standard Model Higgs boson produced in association with a vector boson and decaying to a b-quark pair with the ATLAS detector.
  Phys. Lett. B 718 (2012) 369-390
- 105. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Combined search for the Standard Model Higgs boson in pp collisions at*  $\sqrt{s} = 7$  *TeV with the ATLAS detector*. Phys. Rev. D86 (2012) 032003
- 106. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Measurement of the Lambda\_b lifetime and mass in the ATLAS experiment. Phys. Rev. D 87, 032002 (2013)
- 107. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *A search for ttbar resonances in lepton+jets events with highly boosted top quarks collected in pp collisions at* √s = 7 *TeV with the ATLAS detector*. JHEP 1209 (2012) 041
- 108. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for top and bottom squarks from gluino pair production in final states with missing transverse energy and at least three b-jets with the ATLAS detector. Eur. Phys. J. C72 (2012) 2174

- 109. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for magnetic monopoles in  $\sqrt{s} = 7$  TeV pp collisions with the ATLAS detector. Phys. Rev. Lett 109, 261803 (2012)
- 110. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC. Phys. Lett. B 716 (2012) 1-29
- 111. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Underlying event characteristics and their dependence on jet size of charged-particle jet events in pp collisions at √s = 7 TeV with the ATLAS detector.
  Phys. Rev. D 86 (2012) 072004
- 112. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Time dependent angular analysis of the decay Bs->J/psi phi and extraction of Delta Gamma\_s and the CP-violating weak phase phi\_s by ATLAS.* JHEP 12 (2012) 072
- 113. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for a supersymmetric partner to the top quark in final states with jets and missing transverse momentum at √s = 7 TeV with the ATLAS detector.
  Phys. Rev. Lett. 109, 211802 (2012)
- 114. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurement of WZ Production in Proton-Proton Collisions at* √s = 7 *TeV with the ATLAS Detector*. Eur. Phys. J. C72 (2012) 2173
- 115. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for direct top squark pair production in final states with one isolated lepton, jets, and missing transverse momentum in √s = 7 TeV pp collisions using 4.7 fb<sup>-1</sup> of ATLAS data.
  Phys. Rev. Lett. 109, 211803 (2012)
- 116. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for light scalar top quark pair production in final states with two leptons with the ATLAS detector in √s = 7 TeV proton-proton collisions.
  Eur. Phys. J. C72 (2012) 2237
- 117. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Further search for supersymmetry at  $\sqrt{s} = 7$  TeV in final states with jets, missing transverse momentum and isolated leptons with the ATLAS detector. Phys. Rev. D 86, 092002 (2012)
- 118. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *Measurements of the pseudorapidity dependence of the total transverse energy in proton-proton collisions at* √s = 7 TeV with ATLAS.
  JHEP 11 (2012) 033

- 119. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for Diphoton Events with Large Missing Transverse Momentum in 5 fb<sup>-1</sup> of 7 TeV Proton-Proton Collision Data with the ATLAS Detector.
  Phys. Lett. B 718 (2012) 411-430
- 120. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for high-mass resonances decaying to dilepton final states in pp collisions at √s = 7 TeV with the ATLAS detector.
  JHEP 11 (2012) 138
- 121. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for a heavy top-quark partner in final states with two leptons with the ATLAS detector at the LHC. JHEP 11 (2012) 094
- 122. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C *ATLAS search for a heavy gauge boson decaying to a charged lepton and a neutrino in pp collisions at √s = 7 TeV.* Eur. Phys. J. C72 (2012) 2241
- 123. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for top-jet resonances in the lepton+jets channel of tt + jets events with the ATLAS detector in 4.7 fb<sup>-1</sup> of pp collisions at √s = 7 TeV.
  Phys. Rev. D 86, 091103 (2012)
- 124. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for Supersymmetry in Events with Large Missing Transverse Momentum, Jets, and at Least One Tau Lepton in 7 TeV Proton-Proton Collision Data with the ATLAS Detector. Eur. Phys. J. C72 (2012) 2215
- 125. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for R-parity-violating supersymmetry in events with four or more leptons in s√=7 TeV pp collisions with the ATLAS detector.
  JHEP 12 (2012) 124
- 126. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for anomalous production of prompt like-sign lepton pairs at  $\sqrt{s} = 7$  TeV with the ATLAS detector. JHEP 12 (2012) 007
- 127. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C
  Search for pair production of massive particles decaying into three quarks with the ATLAS detector in √s =7 TeV pp collisions at the LHC.
  JHEP 12 (2012) 086
- 128. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C Search for doubly-charged Higgs bosons in like-sign dilepton final states at √s =7 TeV with the ATLAS detector. Eur. Phys. J. C72 (2012) 2244
- 129. Capua M., Crosetti G., La Rotonda L., Lavorini V., Mastroberardino A., Policicchio A., D. Salvatore, Schioppa M., Susinno G., Tassi E., Atlas C

A Massive Particle Consistent with the Standard Model Higgs Boson observed with the ATLAS Detector at the Large Hadron Collider. Science Vol. 338 no. 6114 pp. 1576-1582

- 130. 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. B 708 (2012) 14-20
- 131. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C Search for Single-Top Production in ep Collisions at HERA. Phys. Lett. B 708 (2012) 27-36
- 132. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C Scaled Momentum Distributions for K<sup>0</sup> s and Lambda/anti-Lambda in DIS at HERA. JHEP 03 (2012) 020
- 133. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C Exclusive Electroproduction of two Pions at HERA. Eur. Phys. J. C 72 (2012) 1869
- 134. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C Inclusive-jet Photoproduction at HERA and determination of Alpha\_s. Nucl. Phys. B864 (2012), pp. 1-37
- 135. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C Search for First-Generation Leptoquarks at HERA. Phys. Rev. D 86, 012005 (2012)
- 136. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C Measurement of isolated photons accompanied by jets in deep inelastic ep scattering. Phys. Lett B. 715 (2012) 88-97
- 137. Capua M., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C Combined inclusive diffractive cross sections measured with forward proton spectrometers in deep inelastic ep scattering at HERA. Eur. Phys. J. C 72 (2012) 2175
- 138. Schioppa M., KLOE-II C Search for a vector gauge boson in phi meson decays with the KLOE detector KLOE-2 Collaboration Phys. Lett. B 706 (2012) 251-255
- La Rotonda L., Policicchio A., Venturelli T., DRC52 Collaboration Detection of electron showers in dual-readout crystal calorimeters Nucl. Instr. and Meth. in Phys. Res. A 686 (2012) 125-135
- 140. La Rotonda L., NOMAD Collaboration A search for single photon events in neutrino interactions Phys. Lett. B 706 (2012) 268-275

### **B PUBLICATIONS ON CONFERENCE PROCEEDINGS B.1 Publications on international conference proceedings in 2012**

 A. Policicchio for the ATLAS Collaboration, Search for New Physics with leptons and/or jets at ATLAS, DOI:10.3204/DESY-PROC-2012-02/199

## PRESENTATIONS AT SCHOOLS AND CONFERENCES

## C.1 Invited presentations at international schools and conferences in 2012

- M. Capua, *Connection between diffraction in DIS and diffraction at the LHC*, Diffraction 2012, Lanzarote, Spain (2012).
- 2. A. Policicchio, Search for new physics with leptons in final state with the ATLAS detector, DIS 2012, Bonn, Germany (2012).
- A. Policicchio, Search for Lepton-Jets with the ATLAS experiment at the LHC, SIF 2012, Napoli, Italy (2012).
- A. Policicchio, Searches for Long-Lived Particles in ATLAS: SUSY+EXOTICS, ATLAS Physics Workshop 2012, Lecce, Italy (2012).
- 5 D. Salvatore,

*Ricerca di decadimenti del bosone di Higgs in particelle "Hidden Valley" con l'esperimento ATLAS a LHC*, SIF 2012, Napoli, Italy (2012).

6 D. Salvatore, Search for long-lived neutral particle de

Search for long-lived neutral particle decays with first 1.94 fb<sup>-1</sup> of data collected in 2011 with the ATLAS detector, HCP 2012, Kyoto, Japan (2012).

- M. Schioppa, *ATLAS searches with non hadronic jets*, Boost 2012, Valencia, Spain (2012).
- 8 E. Tassi, *Inclusive DIS at HERA and PDFs*, Diffraction 2012, Lanzarote, Spain (2012).
- 9 E. Tassi, HERA PDFs, HCP 2012, Kyoto, Japan (2012).

## 6. MOLECULAR BIOPHYSICS

Professors and R	esearchers: Luigi Sportelli		
-	Rosa Bartucci		
	Rita Guzzi		
	Bruno Rizzuti (Lab. LiCryL, IPCF-CNR, UOS Cosenza)		
Post-Doc:	Manuela Pantusa		
PhD Student:	Stefania Evoli		
Technical staff:	Massimo Sposato		
Collaborators:	D. Marsh (MPI for Biophysical Chemistry, Goettingen, Germany)		
	M. Esmann (Aarhus University, Dept. of Biochemistry, Denmark)		
	C. Dennison (Newcastle University, Institute for Cell and Molecular Bioscience, UK)		
	V. Daggett (Washington University, Dept. of Bioengineering)		
	D. E. Otzen, N. Lorenzen (Aarhus University, Dept Mol Biol and i-Nano Centre)		
	F. Bonomi, S. Iametti (Milan University, Department of Food, Environmental and Nutritional		
	Sciences)		
	M.P. De Santo, (Univ. Calabria, Department of Physics and Lab. Licryl, IPCF-CNR, UOS		
	Cosenza)		
	B. Zappone (Lab. Licryl, IPCF-CNR, UOS Cosenza)		
	A. Stirpe (Post-Doc)		
	1 /		

#### Introduction

The research lines carried out by the Molecular Biophysics Group in 2012 are in the framework of structure/dynamics/function relationship in biosystems and concern the following topics: i) transport protein/ligand complexes; ii) aggregation and glassy behavior of proteins; iii) molecular interaction at the lipid/protein interface. A new collaboration in the field of "food biotechnology" started in the last trimester of 2012.

For the first research activity, transport proteins, namely human serum albumin (HSA) and beta-lactoglobulin (beta-LG), complexed with ligands of biomedical interest, namely resveratrol and stearic acids have been considered. Resveratrol is a natural polyphenol that possesses many health benefits, including antioxidant, cardioprotective and anticancer effects, whereas stearic acids are source of energy in cell membranes. The study has been approached by using jointly spectroscopic techniques (both optical absorption and fluorescence) and docking and molecular dynamics simulation.

Proteins are complex systems of great interest in biophysics, whose behavior is highly dependent on environmental conditions of concentration, temperature, pH and ionic strength. They can form aggregates of peculiar features, oligomers of different size and amyloid fibrils likewise evidenced for proteins involved in neurological disorders. Within this context, key features of protein aggregation are addressed by spectroscopic, calorimetric and microscopic approaches.

Similarly, at cryogenic temperature, proteins can show properties found in amorphous systems characteristic of the glassy state. The glass-like state of both small globular model proteins and more large membrane proteins have been characterized via the temperature dependence of the mean-square librational amplitude,  $\langle \alpha^2 \rangle$ , by using spin-label ESR at low temperature.

Finally, the lipid/protein interaction has been investigated in model membranes of anionic DMPG bilayers interacting with alpha-synuclein, a protein related to Parkinson's disease, and in native membranes of Na,K-ATPase, extracted by shark salt gland, by means of continuous wave and pulsed EPR methods of chain-spin labelled lipids.

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

### 6.1 TRANSPORT PROTEIN/LIGAND COMPLEXES

#### 6.1.1 Interaction of resveratrol with transport proteins

Resveratrol is a phenolic compound consisting of two aromatic rings joined by a methylene bridge, naturally found in some plants and thus also in food and beverages, particularly red wine. The *trans*-resveratrol isomer is biologically active and has many health benefits, including antioxidant, cardioprotective and anticancer effects. However, it converts into the inactive *cis*-isomer as a consequence of aging or exposure to UV- and sun-light. In

addition, resveratrol shows limited solubility in aqueous media, leading to poor bioavailability and rapid metabolization in biological fluids. These limitations can be overcome by loading the polyphenol into water soluble carriers.

As potential carriers of *trans*-resveratrol we have considered the two transport proteins, beta-lactoglobulin (beta-LG) and human serum albumin (HSA). The stability of the bound *trans*-resveratrol was compared to the corresponding one in aqueous solution. Spectrophotometry and intrinsic resveratrol fluorescence were used to quantify the fraction of the two isoforms upon continuous illumination with UV light at 340 nm and to study the kinetics of the *trans*-to-*cis* conversion at different temperatures. At molecular level, details of the protein-ligand interaction were obtained by docking calculations and molecular dynamics simulations.

Both the optical absorption and fluorescence results confirm that UV irradiation induces the formation of *cis* isomers in a pure *trans*-resveratrol solution, with the fraction of *trans* isomer further decreasing at increasing temperature. In contrast, when bound to either beta-LG and HSA the stability of resveratrol increases, the latter protein being more effective in protecting resveratrol from degradation. Molecular simulations indicate that the higher efficiency of HSA is due to the location of binding sites for resveratrol in a region constrained and solvent protected, whereas it associates in the central calyx and on an external surface partly exposed to solvent in beta-LG.



Fig. 1. Human serum albumin (left) and beta-lactoglobulin (right) in complex with three and one molecule of trans-resveratrol, respectively.

### 6.1.2 Molecular dynamics and docking of fatty acids interacting with beta-lactoglobulin

Beta-lactoglobulin is the most abundant protein in cow milk, widely studied for its application in food technology. It binds and transports fatty acids of different length and several other ligands. The protein barrel has an open end with a conical shape forming a calyx, which constitutes the primary binding site for hydrophobic molecules. Other binding sites on the external surface have been hypothesized for fatty acids, but their location is debated.

We have used molecular dynamics simulations to investigate the dynamics of saturated fatty acids of different length (8-18 carbon atoms) in the protein calyx. The results indicate that atomic fluctuations in the protein are enhanced when ligands are bound, compared to the apo form. The anchoring of each fatty acid at the entrance of the binding site is provided by electrostatic interactions of the lipid head-group with Lys69 and Lys60 side chains. Interestingly, only the two fatty acids with the longest chain (i.e., palmitic and stearic acid), which experimentally have the highest affinity, are found in a fully extended conformation in simulation.

By combining molecular docking and dynamics simulations, two additional secondary binding sites have been identified for palmitic acid when the main site, i.e. the calyx, is already saturated. One is located in between a helical turn and  $\beta$ -strand B and consists in a small hydrophobic cavity in which the fatty acid molecule partially penetrates, either head-first or tail-first. The other one is located in between the  $\alpha$ -helix and  $\beta$ -strand I and consists in a superficial crevice in which the fatty acid lies in an almost extended conformation.



**Fig. 2.** Beta-lactoglobulin (stick representation, with secondary structure elements of the main chain in transparent representation) with two fatty acid molecules attached (van der Waals representation).

#### 6.2 AGGREGATION AND GLASSY BEHAVIOUR OF MODEL PROTEINS

#### 6.2.1 Effects of the presence of metal ions on the aggregation of beta-lactoglobulin

Low pH, high protein concentration and temperature are suitable experimental conditions to induce spontaneous amyloid-like aggregation and self-assembly of fibrillar nanostructures in beta-lactoglobulin. Transition metal ions are known to affect the amyloid fibrillation and can be used to control the stability and morphology of protein aggregates. In this work, the effect of the presence of Cu(II), Zn(II) and Fe(III) at different concentrations (1:1 and 1:10 protein-to-metal ratio) on the fibrillation of beta-lactoglobulin at pH 2 has been compared with protein structures obtained in the absence of metal. In particular, differential scanning calorimetry (DSC) and atomic force microscopy (AFM) have been used to assess the conformational stability of the protein in solution and the resulting fibril morphology on a surface, respectively.

The results indicate that beta-lactoglobulin in solution is destabilized by the presence of the three metals, as indicated by the reduction of enthalpy in the native to unfolded transition observed in DSC. The effect is weak and similar for Cu(II) and Zn(II), while it is much more marked in the presence of Fe(III) ions. AFM measurements show that beta-lactoglobulin can form multi-strand fibrils with distinct height and periodicity. The statistical mode for the fibril height is 2 nm both in the absence of metals and for Zn(II), and 3 nm for Fe(III). In addition, either of the two height values can be obtained for Cu(II), depending on the metal concentration. The fibril periodicity is about 30 nm for both Zn(II) and Fe(III), whereas it is 64 nm for ribbon-like two-filament fibrils that can be obtained in the presence of Cu(II).

The overall findings suggest the possibility to control the size and shape of fibrillar aggregates of betalactoglobulin by modulating the amount and type of transition metal ions in solution.



**Fig. 3.** Models of periodic multi-strand protein fibrils produced by the aggregation of aperiodic protofilaments.  $1^{st}$  order fibril is a single protofilament of thickness h;  $2^{nd}$  and  $3^{rd}$  order fibrils are twisted bundles containing n protofilaments with periodicity  $p_{n}$ .

### 6.2.2 Glassy behavior of proteins

Librational motions in the region of the protein "glass" transition are analysed for spin-labelled haemoglobin, human serum albumin and beta-lactoglobulin by EPR spectroscopy. A discontinuity in the temperature dependence of the mean-square librational amplitude,  $\langle \alpha^2 \rangle$ , occurs in the region of 200 K as found for the mean-square atomic displacement,  $\langle r^2 \rangle$ , at the protein dynamic transition by Mössbauer spectroscopy and neutron scattering. The discontinuity in  $\langle \alpha^2 \rangle$  vs. *T* can be described by the Vogel-Tamman-Fulcher equation, implying a finite glass transition temperature. Above the dynamic transition,  $\langle \alpha^2 \rangle$  vs. 1/*T* can be approximated by the Arrhenius law with activation energies similar to those usually found for  $\langle r^2 \rangle$ , and  $\beta$ -relaxation in glass-forming media and the hydration shells of proteins. Similar results are found for librational fluctuations of membranous Na,K-ATPase spinlabelled either on superficial –SH groups or on those essential to activity.

## 6.3 MOLECULAR INTERACTION AT THE LIPID/PROTEIN INTERFACE

#### 6.3.1 Association of alpha-synuclein and mutants with lipid membranes

Alpha-synuclein (aSN) is a small soluble presynaptic protein (140 residues) involved in several forms of neurodegenerative disease and is the major component of the pathological lesions associated with Parkinson's disease. It is natively unfolded in solution, assumes amyloid structures spontaneously, and acquires secondary structure upon interaction with lipid membranes.

We use electron spin resonance (ESR) spectroscopy of chain-labelled phospholipids to characterize the interaction of wild-type wt-aSN and mutants with dimyristoylphosphatidylglycerol (DMPG) extruded unilamellar vesicles (average diameter 200 nm). Three mutants in the N-terminal domain (residues 1-102) are considered in this study, namely A30P, E46K and A53T, which are linked independently to early-onset familial Parkinson's disease.

wt-aSN associates on the negatively charged surface of DMPG vesicles, reduces the mobility (i.e., increases the chain order) in the upper part of the lipid chains in the fluid phase, does not perturb the lipid chain packing at the hydrophobic core of the bilayer and leaves almost unperturbed the main phase transition of DMPG membranes at Tm  $\approx 22$  °C.

The mutants induce chain order at the polar/apolar interface both in the gel and fluid phase of DMPG vesicles and affect the characteristics of the main transition by increasing of about 2 °C the temperature and the cooperativity of the transition relative to DMPG/wt-aSN complex.

### 6.3.2 Water penetration profile at the protein-lipid interface in Na,K-ATPase membranes

The affinity of ionized fatty acids for the Na,K-ATPase has been used to determine the transmembrane profile of water penetration at the protein-lipid interface. The standardized intensity of the electron spin echo envelope modulation (ESEEM) from <sup>2</sup>H-hyperfine interaction with D<sub>2</sub>O was determined for stearic acid, *n*-SASL, spinlabelled systematically at the C-*n* atoms throughout the chain. In both native Na,K-ATPase membranes from shark salt gland and bilayers of the extracted membrane lipids, the D<sub>2</sub>O-ESEEM intensities of fully charged n-SASL decrease progressively with position down the fatty acid chain towards the terminal methyl group. Whereas the D<sub>2</sub>O intensities decrease sharply at the *n*=9 position in the lipid bilayers, a much broader transition region in the range *n*=6 to 10 is found with Na,K-ATPase membranes. Correction for the bilayer population in the membranes yields the D<sub>2</sub>O-intensity profile at the protein-lipid interface. For each chain position, the D<sub>2</sub>O concentrations at the interface are greater than in the lipid bilayer, and the positional profile is much broader. In particular, there is a significant water concentration at the membrane mid-plane adjacent to the protein, unlike the situation in the bilayer regions of this cholesterol-containing membrane. Experiments with protonated fatty acid and phosphatidylcholine spin labels, both of which have a considerably lower affinity for the Na,K-ATPase, confirm these results.



**Fig. 4.** Schematic representation of membrane-bound Na,K-ATPase enzyme (left) and transmembrane water penetration profile (right) as detected by the dependence of  $D_2O$ -ESEEM amplitude on position, n, in the chain of spin-labelled stearic acid (n-SASL).

## 6.3.3 Protein marker in food biotechnology

Shelf-life of food is highly dependent on the storage and packaging conditions. For meet storage, polymeric films with a controlled gas permeability are commonly used to avoid degradation and discoloration.

The research program concerns the evaluation of the stability of muscle beef packaged in oxygen permeable wrapped-tray units and stored in a new master-bag system, with and without oxygen scavengers. Cw-EPR measurements were performed either on fresh meet samples or in samples stored up to seven days in the master-bag. Preliminary results indicate that the intensity of the Fe(III)-heme bound to myoglobin correlates with the storage condition being higher under anoxic atmosphere.

## A PUBLICATIONS ON SCIENTIFIC JOURNALS

A.1 Publications on international journals

## A.1.1 Publications on international journals printed in 2012

- R. Guzzi, B. Rizzuti, R. Bartucci Dynamics and Binding Affinity of Spin-Labeled Stearic Acids in β-Lactoglobulin: Evidences from EPR Spectroscopy and Molecular Dynamics Simulation J. Phys. Chem. B 116 (2012) 11608–11615.
- M. Pantusa, L. Sportelli, R. Bartucci Influence of stearic acids on resveratrol-HSA interaction Eur. Biophys. J. 41 (2012) 969–977.
- 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. 512 (2012) 18-23.

### A.1.2 Publications on international journals accepted in 2012

- B. Zappone, M. P. De Santo, C. Labate, B. Rizzuti, R. Guzzi Catalytic activity of copper ions in the amyloid fibrillation of β-lactoglobulin Soft Matter Accepted (2012) doi: 10.1039/c2sm27408fi
- B. Rizzuti, V. Daggett Using simulations to provide the framework for experimental protein folding studies Arch. Biochem. Biophys. Accepted (2012) doi: 10.1016/j.abb.2012.12.015

### A.1.3 Publications on international journals submitted in 2012

- D. Marsh, R. Bartucci, R. Guzzi, L. Sportelli, M. Esmann Librational fluctuations in protein glasses Biochim. Biophys. Acta – Proteins. Submitted (2012)
- 2. R. Guzzi, R. Bartucci, D. Marsh Heterogeneity of protein substates visualised by spin-label EPR Biophys. J. Submitted (2012)
- 3. R. Bartucci, R. Guzzi, L. Sportelli, M. Esmann D. Marsh *Water penetration profiles at the protein-lipid interface in Na,K-ATPase membranes* Biophys. J. Submitted (2012)
- 4. S. Evoli, R. Guzzi, B. Rizzuti Dynamics and unfolding pathway of chimeric azurin variants: insights from molecular dynamics simulation J. Biol. Inorg. Chem. Submitted (2012)
- M. Pantusa, R. Bartucci, B. Rizzuti Stabilizing effect of transport proteins on the trans-to-cis conversion of resveratrol J. Phys. Chem. B Submitted (2012)

## C INVITED PRESENTATIONS

## C.1 Invited presentations at international conferences in 2012

1. R. Bartucci Polarity and water accessibility in biosystems: continuous-wave versus pulsed EPR SIF 2012 - 98th National Congress of Italian Physics Society, Napoli, 17-21 September 2012

### D PRESENTATIONS AT CONFERENCES

## D.1 Presentations at international conferences in 2012

## D.2 Presentations at national conferences in 2012

- S. Evoli, R. Guzzi, L. Sportelli, B. Rizzuti *Molecular dynamics of chimeric cupredoxins*  IPCF 2012 – First General Meeting of the Italian Institute for Chemical-Physical Processes Cetraro (CS), 21-23 May 2012
- B. Rizzuti, R. Bartucci, L. Sportelli, R. Guzzi Binding mechanism for naturally-occurring and spin-labeled fatty acids in transport proteins IPCF 2012 – First General Meeting of the Italian Institute for Chemical-Physical Processes Cetraro (CS), 21-23 May 2012
- C. Labate, B. Zappone, M.P. De Santo, B. Rizzuti, R. Guzzi *Catalytic activity of copper ions in the amyloid fibrillation of β-lactoglobulin* IPCF 2012 - First General Meeting of the Italian Institute for Chemical-Physical Processes Cetraro (CS), 21-23 May 2012
- M. Pantusa, R. Bartucci Binding of the antioxidant polyphenol resveratrol to human serum albumin. Influence of stearic acids pre-complexed with the protein IPCF 2012 - First General Meeting of the Italian Institute for Chemical-Physical Processes Cetraro (CS), 21-23 May 2012
- M. Pantusa, L. Sportelli, R. Bartucci *Stearic acids influence resveratrol-HSA interaction* SIF 2012 - 98th National Congress of Italian Physics Society, Napoli, 17-21 September 2012
- S. Evoli, R. Guzzi, B. Rizzuti Molecular dynamics of azurin: comparison with azu-amicyanin and azu-plastocyanin mutants SIF 2012 - 98th National Congress of Italian Physics Society, Napoli, 17-21 September 2012
- M. Pantusa, L. Sportelli, R. Bartucci *Influence of stearic acids bound to HSA on the Resveratrol-HSA interaction* SIBPA 2012 - XXI National Congress of the Pure and Applied Biophysics Society, Ferrara, 17-20 September 2012
- B. Rizzuti, R. Guzzi, R. Bartucci *The role of binding site hydration in fatty acid coordination with β-lactoglobulin* SIBPA 2012 - XXI National Congress of the Pure and Applied Biophysics Society, Ferrara, 17-20 September 2012
- S. Evoli, R. Guzzi, L. Sportelli, B. Rizzuti Dynamical role of the metal binding loop in active site-engineered blue copper proteins SIBPA 2012 - XXI National Congress of the Pure and Applied Biophysics Society, Ferrara, 17-20 September 2012
- R. Guzzi, B. Rizzuti, C. Labate, M.P. De Santo, B. Zappone *Fibrillar aggregation of β-lactoglobulin in the presence of copper ions* SIBPA 2012 - XXI National Congress of the Pure and Applied Biophysics Society, Ferrara, 17-20 September 2012

# 7. PHYSICS AND APPLICATIONS OF THE SOFT MATTER

Professors and	
Researchers	Roberto Bartolino
	Riccardo C. Barberi
	Enzo Cazzanelli
	Gabriella Cipparrone
	Maria Penelope De Santo
	Pasquale Pagliusi
	Nicola Scaramuzza
	Giuseppe Strangi
	Roberto Caputo
	Cesare Umeton
	Carlo Consolato Versace
	Antonio De Luca
Personnel of the	Federica Ciuchi (IPCF-CNR, UOS DI Cosenza, Italy)
	Michele Giocondo (IPCF-CNR, UOS DI Cosenza, Italy)
Licryl lab	Giuseppe Lombardo (IPCF-CNR, UOS DI Cosenza, Italy)
·	Alfredo Mazzulla (IPCF-CNR, UOS DI Cosenza, Italy)
	Bruno Zappone (IPCF-CNR, UOS DI Cosenza, Italy)
	Alfredo Pane (IPCF-CNR, UOS DI Cosenza, Italy)
	Fernanda Annesi (IPCF-CNR, UOS DI Cosenza, Italy)
Postdoc fellows	Emanuela Bruno
	Marco Castriota
	Melissa Infusino
	Gia Petriashvili
	Luigia Pezzi
	Clementina Provenzano
	Corona Ruiz
	Salvatore Marino
	Luciano De Sio
	Hari Krishna Koduru
PhD students	Lucia Marino
	Ugo Cataldi
	Iryna Gryn
	Rakes Dhama
	Alireza R. Rashed
	Angela Fasanella
	Raul Josue Hernandez
	Eugenia Lepera
	Dariia Lysenko
	Navinkumar J. Patil
Collaborators	Massimo Sposoto (Università della Calabria, Cosenza, Italy)
Conuborators	Massino sposato ( <i>Universita della Calabria</i> , Cosenza, Italy)
International	
collaborations	
condorations	LPCM-IPCF-CNR LIOS DI S University Bordeaux I (France) Center for Bio-
	Molecular Science and Engineering Naval Research Lab Washington D C (USA)
	Bulgarian Academy of Sciences Sofia (Bulgaria)
	Laboratory of Nanotechnology UCLM (Sprain)
	Department of Chemistry Moscow State University (Dussia)
	Centre Paul Pascal - Bordeaux (France)
	University of Colorado - Boulder (USA)
	Onversity of Colorado - Dounder (OSA)
	0.4

University of Tunis (Tunisia) College de France - Paris (France) University of Marseille (France) Chalmers University - Goteborg (Sweden) University of Kent (USA) Polytechnic of Madrid (Spain) Polytechnic of Bucharest (Romania) University of Gent (Belgium) University of Ljublijana (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) FBK Foundation of Trento (Italv) Dipartimento di Scienze e Ingegneria della Materia, dell' Ambiente ed Urbanistica Università Politecnica delle Marche (Italy) University of Oxford (UK) Department of Environmental and Chemical Engineering, University of Calabria; and Consorzio INSTM (Italy) Department of Chemistry, University of Calabria (Italy) Departamento de Fisica, Universidade Estadual de Maringa (Brazil) University of California Santa Barbara (USA) University of Massachusetts, Lowell (USA) Institut de Nanosciences de Paris (INSP) (France) Nanyang Technological University (NTU) (Singapore) Denmark Technological University, Copenaghen (Denmark) Dipartimento di Informatica, Università degli Studi di Verona ((Italy) IMEM-CNR Istituto dei Materiali per l' Elettronica ed il Magnetismo CNR, Parma (Italy) FBK-(Povo) Trento (Italv) Istituto di Fotonica e Nanotecnologie, Sezione di Trento (Italy) Institute of Solid State Physics, University of Latvia (Lettland) Department of Chemistry and Biochemistry, University of Tulsa, Oklahoma (USA) Ecole Polytechnique Federal de Lausanne, Institute of Microtechnology, Optics and Photonics Technology (Switzerland) University of Hull, Department of Chemistry, Liquid crystal and advanced organic materials group (UK)University Jena, Institute for Condensed Matter Theory and Solid State Optic (Germany) University of Patras, Department of Materials Science, Molecular theory group (Greece) The University of Sheffield, Polymers, Liquid Crystals and Supramolecular Structures Group (UK)Virtual Institute for Artificial Electromagnetic Materials and Metamaterials - METAMORPHOSE VI AISBL, University of Geneva, Physical Chemistry Department, Surfaces Chemistry and Nanosciences Laboratory (Switzerland) Laboratorio di Genetica, Università della Calabria (Italy) Université Paris Diderot (France) PMMH (France) LIMSI, CNRS (France) UPMC Université Paris 06 (France) CNRS, Ecole Normale Super, Lab Phys Stat (France) Novosibirsk State University (Russia)

Institute of Geology and Mineralogy, SB RAS, Novosibirsk (Russia) Rzhanov Institute of Semiconductor Physics, SB RAS, Novosibirsk (Russia) Boreskov Institute of Catalysis, SB RAS, Novosibirsk (Russia) Institute of Strength Physics and Materials Science, Tomsk (Russia) Donostia International Physics Center (DIPC), San Sebastian/Donostia (Spain) Departamento de Fisica de Materiales UPV/EHU, Centro de Fisica de Materiale (Spain) Dipartimento di Chimica, Università di Sassari (Italy) Materials Engineering Centre, Università di Perugia, INSTM, NIPLAB, Terni (Italy) Dipartimento DISIT, Università del Piemonte Orientale "A. Avogadro", INSTM, UdR Alessandria (Italv) CEMIF.CAL Rende, Cosenza (Italy) P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow (Russia) Dipartimento di Chimica e Chimica Industriale, Università di Pisa, INSTM, UdR Pisa (Italy) Faculty of Physics, University of Bucharest (Romania) Faculty of Applied Sciences, University Politehnica of Bucharest (Romania) Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia (Bulgaria) Group of Nanotechnology and Materials, UCLM, Laboratory of Nanotechnology, Almaden (Spain) Srivenkateswara University, Tirupati, Andhra Pradesh (India) Dipartimento di Fisica and CNISM, Politecnico di Torino (Italy) Institute of Cybernetics of Georgian Academy of Science, Tbilisi (Republic of Georgia) University of Vigo (Spain) CNRS - Centre National de Recherche Scientifique, Bordeaux – Paris (France) CNR-IPCF (UOS Cosenza – UOS Bari) (Italy) University of Manchester (UK) Helsinki University of Technology (Finland) Université Catholique de Louvain (Belgium) Università degli studi di Siena (Italy) Fraunhofer Gesellschaft zur Förderung der angewandten Forschung e. V. (Germany) Rhodia LOF (France) Case Western Reserve University, Ohio (USA) Instituto Nacional de Astrofísica, Óptica y Electrónica, Puebla (Mexico) Universidad Nacional Autonoma de Mexico, Mexico City (Mexico) Institute of Physics, National Academy of Science of Ukraine, Kiev (Ukraine) Dept. of Electronic and Computer Engineering, Hong Kong University of Science and Technoligies (Hong Kong) JASCO Europe srl, e Dipartimento di Scienze Biomediche e Biotecnologie, Università di Brescia (Italy)

### 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, biological-syntetic). 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 Application of Raman spectroscopy to the characterization of solids, thin films, soft matter, as well as artifacts of cultural heritage

In particular, during the 2012, have been published works about the composite system POLYCRIPS (polymer+ nematic liquid crystals), related to the NANOGOLD European project.

Samples of graphene, deposited by CVD of ethylene on Pt(111) surface, have been investigated, by using, among different techniques, the micro-Raman spectroscopy, and some results have been presented in national and international conferences. This activity is related to a FIRB project.

An investigation on a oil painting of Neapolitan anonymus, attributed by the art critics to the Baroque age, has been carried out.

Finally, other works, connected to the collaboration with the CNR group of Trento and the University of Verona, have been published, concerning, respectively, the application of organic thin film deposition to the sensor technology and the basic Raman spectroscopic research on the crystals.



The painting "*Rebecca at the well*" has been kindly provided for this study by the "Museo dell'Ottocento e del Novecento" of Rende. A remarkable finding in this investigation is the spectroscopic evidence of a modern migment, Cuphthalocianine, used for some restoration not recorded in written documents. This research has been published on Journal of Raman spectroscopy



*Micro* -*Raman* evidence of a preferential orientation of the NLC director within the POLICRYPS structure: at  $\theta = 90^\circ$ , the *Raman* intensities show a maximum because the director n is parallel to the polarization direction of the laser light



*Micro-Raman spectra from different spots of monolayer graphene on Pt(111), collected along a line and spaced of about 10 micron. Values of bandwidth are reported for both the G band at 1600 cm<sup>-1</sup> and the 2D overtone at about 2700 cm<sup>-1</sup>* 

# 7.1.2 Non-Debye relaxation in the dielectric response of nematic liquid crystals: Surface and memory effects in the adsorption-desorption process of ionic impurities

We demonstrate theoretically that the presence of ions in insulating materials such as nematic liquid crystals may be responsible for the dielectric spectroscopy behavior observed experimentally. It is shown that, at low frequencies, an essentially non-Debye relaxation process takes place due to surface effects. This is accomplished by investigating the effects of the adsorption-desorption process on the electrical response of an electrolytic cell when the generation and recombination of ions is present. The adsorption-desorption is governed by a non-usual kinetic equation in order to incorporate memory effects related to a non-Debye relaxation and the roughness of the surface. The analysis is carried out by searching for solutions to the drift-diffusion equation that satisfy the Poisson equation relating the effective electric field to the net charge density. We also discuss the effect of the mobility of the ions, i.e., situations with equal and different diffusion coefficients for positive and negative ions, on the impedance and obtain an exact expression for the admittance. The model is compared with experimental results measured for the impedance of a nematic liquid crystal sample and a very good agreement is obtained.

# 7.1.3 Fractional Diffusion Equation and the Electrical Impedance: Experimental Evidence in Liquid-Crystalline Cells

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.



*Real (R) and imaginary (X) parts of the electrical impedance of the cell versus the frequency of the applied voltage, f* =  $\omega/2\pi$ .

## 7.1.4 Dielectric investigations on new bent-core liquid crystal

Dielectric measurements on a bent-core liquid crystal were carried out in the frequency range from 10 mHz to 100 kHz in planar aligned cells. Four relaxation ranges were detected during heating condition: two in a low frequency range of a few hertz probably due to conductivity and interface relaxation phenomena, another between 10 and 20 Hz, and another one in a range between 10 kHz and 100 kHz in smectic as in nematic and isotropic phases. The third relaxation response is no more visible during cooling conditions. Dielectric increments, distribution parameters, and relaxation frequencies have been evaluated at different temperatures by fitting data with Havriliak- Negami (H-N) relaxation function, which is an empirical modification of the Debye relaxation model. The presence of a relaxation response between 10 and 20 Hz and the relatively great values of the permittivity could suggest the presence of a ferroelectric response due to the presence of cybotactic clusters.

## 7.1.5 Dielectric Characterisation of 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.

### 7.1.6 Flexoelectro-Optical Behaviour of Layers Formed by Polymer-Liquid Crystal Phase-Separated Composites

The flexoelectro-optical behavior of layers formed by a liquid crystal (LC)-polymer phase-separated composite was investigated by flexoelectric spectroscopy. The composite layers with a thickness of 6  $\mu$ m contain micrometer-sized droplets of LC E7 dispersed in a transparent polymer matrix. The layers were prepared between glass substrates with Teflon nanolayers initially deposited. Thus, LC-polymer composite layers with well ordered and aligned droplet morphology were obtained. The dispersed LC droplets were spherical in shape, with a mean size of about 14  $\mu$ m. The flexoelectric response of LC droplets in this structure was studied as depending on both temperature and applied voltage.

# 7.1.7 Tailoring the physical properties of polymeric nanocomposite films by the insertion of graphene and metal nanoparticles

New polymeric nanocomposite films containing graphene and metal nanoparticles were synthesized and their morphological, thermal, surface and dielectric properties were studied. These materials present interesting characteristics that make them suitable for different applications. For example, the wetting property can be tuned by the insertion of nanofillers. The presence of nanofillers also increases the dielectric strength of the polymer films.



*Raman spectra of graphene obtained from filtration of TEGDA/graphene dispersion (0.05 wt.-%) (bottom line), and graphite (top line)* 



TEM images of TEGDA/graphene dispersion



Sessile drop of water on (a) PTEGDA+graphene and (b) PTEGDA+graphene+Au samples. The contact angle is evaluated by fits carried out in the framework of the Young-Laplace's theory.

# 7.1.8 Ferroelectric switching in the cybotactic nematic phase of a main-chain liquid crystal polymer with bent-core monomeric unit

We report the first example of ferroelectric switching in the nematic phase of a bent-core liquid crystal polymer. We measured a significant polarization of 0.85  $\mu$ C cm-2 upon application of an electric filed of only 1 V  $\mu$ m-1. The effect is ascribed to the field-induced alignment of polar cybotactic clusters, whose presence is revealed by X-ray diffraction.



LA-XRD patterns of **II** collected on (A-F) heating and (G-K) cooling the sample under a horizontal aligning **B** field. (L) Temperature dependence of the XRD structural parameters on heating (empty symbols) and cooling (full symbols): *d* is the layer spacing (black squares),  $\beta$  the tilt angle (blue triangles), and  $L = d/\cos\beta$  the calculated molecular length (red circles).



(A-F) WA-XRD diffraction patterns of **II** collected on cooling from the Ncyb phase (T = 230 °C) under a horizontal aligning **B** field; because of the symmetry of the pattern, only the upper half is entirely shown. (G) Corresponding q-scans obtained by azimuthal integration



Repolarization current response in the Ncyb phase of II (black solid line) measured on a 30  $\mu$ m-tick cell at 248 °C upon application of a triangular wave voltage (f = 1 Hz, Vpp = 60 V, grey dotted line). The two arrows indicate the current peaks associated with the polarization switching

### 7.1.9 Shaping supramolecular chirality in smart polymers with 2D Polarization Light Patterns

Supramolecular chiral periodic structuring of an amorphous azo-polymer is demonstrated, exploiting the sensitivity of the material 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.



# 7.1.10 Programmable microlens arrays by single-step polarization holographic recording in photosensitive soft materials

The optical microsystems have become important tools for imaging, optofluidics and sensors applications. Here we show a versatile method to create microlens arrays (MAs) exploiting the spatial light modulator (SLM) assisted polarization holography, which enables an efficiency of diffraction up to 100%. We demonstrate the large flexibility of the proposed approach by codifying mixed MAs, i.e. composed of spherical and cylindrical lenses with different focal lengths, either positive or negative. Reconfigurable MAs with 70% total diffraction efficiency have been



recorded on a photosensitive polymer that exhibits linear photoinduced birefringence with long time stability as well as optical and thermal reversibility. The good quality of the microlenses array has been shown by a digital holographic test.

## 7.1.11 Chiral Self-assembled solid microparticles

Recently we have developed a method to create solid chiral microparticles. They are spherical particles where the chirality is present both at the molecular level and at the supramolecular level, organizing helical structures confined in region with different geometries (spherical, conical and cylindrical) inside the particle. The chiral solid microparticles were obtained by exploiting light-induced polymerization of cholesteric liquid crystal droplets in water emulsion. The polymeric beads preserve the supramolecular structures of the precursor cholesteric droplets. The self-organized internal configurations depend on the characteristic lengths of the system, namely the dimension of particles and the spatial periodicity of the helical structures. The addition of a surfactant in the water emulsion promotes the perpendicular orientation of the liquid crystal molecules at the water interface of the precursor droplet and modifies the arrangement of the supramolecular structures. Some applications in the field of optical manipulation and photonics that make evidence of their unique properties are investigated.



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

## 7.2.1 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/µm. Concerning this structure, in the period of observation (2011), 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.

### 7.2.2 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.



SEM view of the emptied polymer matrix to be used as a fillable template

### 7.2.3 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.

### 7.2.4 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.



POM view of the polymeric template filled with CLC and Au NPs mixture at the edge of the grating area (a). The high magnification of the CLC and Au NPs area aligned in ULH geometry is shown in (b) while its typical reflection notch is reported in (c). EBSD view (d) and high magnification (e) of the polymeric template filled with CLC and Au NPs

### 7.2.5 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 Buergi of the University of Geneva.



Wavelength of the plasmon resonances versus the applied strain; the dash lines indicate the points of minimum of the surface plasmon resonances

### 7.2.6 Electro-switchable soft materials for photonic applications

We report on the fabrication and characterization of a new generation of electro-switchable optofluidic devices based on flexible substrates, combined with the extraordinary properties of reconfigurable soft-materials. A conductive polydimethylsiloxane microstructure has been first sputtered with an Indium Tin Oxide (ITO) layer and then functionalized with an amorphous film of SiOx. Then, the "layer" by "layer" microstructure has been infiltrated with an anisotropic and reconfigurable fluid (Nematic Liquid Crystal, NLC). The sample has been characterized in terms of morphological, optical and electro-optical properties: the soft-conductive microstructure exhibits a uniform and regular morphology, even after testing with mechanical stretching and deformations. Combination of the conductive ITO with the functionalization film (which has been employed for inducing in-plane alignment of NLC molecules) enables us to carry out a series of optical and electrooptical experiments; these confirm excellent properties in terms of a reconfigurable device and a diffractive element as well.



A SEM view of the ITO sputtered PDMS microstructure (a) and its high magnification (b) after deformation tests (c). A SEM view of the microstructure after evaporating SiOx on the ITO layer (d) and its high magnification (e). A sketch of the NLC configuration (f) in the aligning, electro-conductive, PDMS cell (g). A POM view of the grating area containing the NLC with its molecular director axis at 45u (h) and 0u (i) with respect to the polarizer axis

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

#### 7.3.1 Loss Compensation Routes in Metamaterials Sub-Units

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.



7.3.2 Polymer based Diffraction gratings

This work was devoted to obtain the first realization and characterization of two-dimensional periodic and aperiodic POLICRYPS (Polymer Liquid Crystal Polymer Slices) structures, obtained by means of a single-beam holographic technique exploiting a high resolution spatial light modulator (SLM). A first investigation shows that the gratings, operating in the Raman Nath regime, exhibit a morphology and a electro-optical behavior that are typical of the POLICRYPS gratings realized by two-beam interference holography.

We exploited the use of a reflective Spatial Light Modulator (SLM); the main feature of this device is that it can modify the wavefront of an impinging laser beam in such a way that any desired two dimensional light pattern can be obtained. Some of these patterns are impossible to be realized by using standard interference holography; on the contrary, they can be obtained by just reconfiguring, in real time, the SLM display. In the following, we report on the attempts done to fabricate some 2D POLICRYPS structures by utilizing the new procedure, along with related electro-optical characterization experiments. A valid example of this new scenario of possibilities is the realization of a fork grating that, at our knowledge, is impossible to be realized by using standard holographic techniques. The electro-optical characterization of all fabricated structures shows the typical behavior of the POLICRYPS ones. This promising result put the basis for a further development and optimization of the technique.



Another research activity concerned with the fabrication and characterization of a new generation of electroswitchable optofluidic devices based on flexible substrates, combined with the extraordinary properties of reconfigurable soft-materials. A conductive polydimethylsiloxane microstructure has been first sputtered with an Indium Tin Oxide (ITO) layer and then functionalized with an amorphous film of SiOx. Then, the "layer" by "layer" microstructure has been infiltrated with an anisotropic and reconfigurable fluid (Nematic Liquid Crystal, NLC). The sample has been characterized in terms of morphological, optical and electro-optical properties: the soft-conductive microstructure exhibits a uniform and regular morphology, even after testing with mechanical stretching and deformations.

Combination of the conductive ITO with the functionalization film (which has been employed for inducing in-plane alignment of NLC molecules) enables us to carry out a series of optical and electrooptical experiments; these confirm excellent properties in terms of a reconfigurable device and a diffractive element as well.



7.3.3 Study of microparticles with anisotropic optical properties and also chiral, that combines the science of soft matter photonics and optical manipulation

The particles, carried by the control of both the internal structure and surface properties, constitute microresonators spherical suitable for various applications such as the lasing. These have allowed the implementation of new strategies for optical trapping.



Optical microscope images of microspheres chiral

# 7.3.4 Lasing in photonic bandgap materials based on liquid crystals doped with fluorescent dyes in liquid crystalline phases (cholesteric blue-phase)

Realization of strategies for tunability in wavelength by the use of principles such as the application of external electric fields, the control of temperature and the concentration of the chiral component.

## 7.3.5 Generation of complex beams by means of polarization holograms

The experimental generation of complex beams by means of a polarization holographic technique has been investigated. The interference of a reference Gaussian beam and a complex beam having opposite circular polarization states, stored on a highly polarization sensitive material, generates polarization holograms whose diffracted beams are high quality complex fields. The technique is tested with the generation of three different types of beams: a simple vortex, a Bessel and a Laguerre-Gaussian beam. This suggests an alternative method for the generation of complex beams with predetermined polarization states.



## 7.3.6 Liquid Crystal Based Polarization Gratings for Spectro-Polarimetric Applications

Two approaches to produce near-ideal Cycloidal Optical Axis Gratings (OAGs) based on liquid crystalline materials have been developed. Both methods rely on polarization holograms recorded on the photoaligning substrates for liquid crystal devices. In the first case, a nematic LC layer, made of low molar mass mesogens, is confined between two parallel substrates, both imposing spatially periodic planar alignment. In the second case, a reactive mesogen (RM) is coated on a single aligning substrate. The unique polarization properties of the OAG have been exploited for the development of a photopolarimeter and a real time and artifact-free circular dichroism spectrograph.



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

### 7.4.1 Periodic Defect Patterns And Guided Nanoparticle Assembly In Smectic Liquid Crystal Films

Continuing our work on the effect of strong confinement on liquid crystal films subject to conflicting boundary conditions [1], we are studying periodic micropatterns that spontaneously appear in smectic films due to the nucleation and self-assembly of defect domains [2]. The domain dimensionality (1D/2D), symmetry and size, ranging from less than 0.5  $\mu$ m to several  $\mu$ m, can be controlled by varying the film thickness and boundary conditions (anchoring), and applying an

external electric field. Smectic micropatterns are useful for various applications, such as templates for soft lithography and microlens arrays, where pattern regularity over large areas, rapid self-assembly and a 'soft' responsive character are demanded.



We focus on the ability of such micropatterns to organize the spatial distribution of nanoparticle dispersions owing to a strong interaction between nanoparticles and the *core* of liquid crystal defects. Namely, 1D patterns induce the formation of *nanochains* trapped within linear defects with a cross-sectional size comparable to the nanoparticle diameter [3]. Moreover, chains of gold nanoparticles show polarization-dependent optical plasmon resonance due to optical coupling of nanoparticles along the chains. Understanding nanoparticle-defect interactions is complicated by the lack of knowledge on the nanoscale structure of the defect domains. By combining the results of synchrotron X-ray diffraction, polarized fluorescence confocal microscopy and atomic force microscopy, we have showed that defect domains and patterns are the result of a complex balance between boundary interactions and distortions of the smectic layered structure, achieved through anchoring and structure frustrations and/or creation of uncommon defect types such as curvature walls and virtual singularities. This work is being developed in collaboration with E. Lacaze at the Paris Institut for Nanoscience (INSP) and University of Paris 6.

### 7.4.2 Nanoscience and biomedicine

Plasmonic photothermal therapy (PPTT) is a minimally-invasive oncological treatment strategy in which photon energy is selectively administered and converted into heat sufficient to induce cellular hyperthermia. To this end, Plasmonic metallic nanoparticles (NPs) are a particular class of nanomaterials which possess the capability to localize light down to the nanoscale by exploiting a phenomenon called Localized Plasmon Resonance (LPR). NPs have been used in therapeutics by triggering drug release or enhancing ablation of diseased tissues, while minimizing damage to healthy tissues. In the framework with the Genetic laboratory (University of Calabria) we have performed a Scanning Electron-Microscopy (SEM) characterization of an immortal cell line used in scientific research called "*HeLa cell*". The breakthrough idea is based on the possibility to deliver NPs in the tumor site and by exploiting the efficient conversion of Near Infrared (NIR) light to heat opens up a new "drug-free" cancer therapy.

Gene delivery is the process of introducing foreign DNA, RNA into host cells as potential therapeutic strategies for various diseases by means of a nano-vehicle. In particular, the properties of an ideal non-viral vector are: low degradation, target specific cells avoiding immune response in the patient. One of the most promising alternative technologies for gene theraphy is the use of NPs as delivery vehicles. The optical properties of NPs and their biocompatibility provide an efficient tool like non-viral vector for gene therapy. We have combined NPs and a human whole genomic DNA exploiting the possibility to realize applications on the Plasmonic Gene Theraphy (PGT). We have characterized the interaction between

NPs and nucleic acids of different length by using analytical techniques, such as electrophoretic mobility assay and scanning electron-microscopy.

In collaboration with Biochemical laboratory (University of Calabria) and ENEA, (Trisaia Research Center, S.S. 106 Jonica, Rotondella, Matera, Italy), we have exploited the possibility to deliver genetic materials to *Solanum lycopersicum* and *Pinus* by using NPs as active vehicle. In a first attempt, we have performed microfluidic experiments devoted to optimize the NPs concentration. Therefore, the presence of NPs within the leaves have been checked my means of spectroscopic and morphological analysis.

In collaboration with laboratory of Genetics and the CTC Department - University of Calabria, we performed a cellular study to better understand the mechanism of action of some molecules that could have therapeutic action useful in the treatment of some hereditary diseases of the nervous system. Subsequently, will be evaluated the effects of molecules on cell cultures by the analysis of the expression of certain genes involved in the mechanisms neurodegeneration.

### 7.4.3 Nanomechanics and nanotribology of adhesive and lubricating protein layers

The CNR group at the Department of Physics has recently upgraded the Surface Force Apparatus (SFA) with a new module that allows accurate nanoscale measurements of the separation, contact geometry, normal forces and friction between two macroscopic surfaces.

The SFA is currently being used to study the nanomechanics and nanotribology (boundary lubrication) of adsorbed protein layers with special adhesive or lubricating properties in aqueous media. We focus on mucins, providing protection and lubrication on most wet surfaces in the body of vertebrate animals, and Perna Viridis mussel foot proteins, used by sea mussels to adhere to rock under water. These proteins are provided in purified form through collaborations with the Denmark Technical University and Singapore Nanyang Technical University, respectively. The goal of our study is to clarify how the enhancement or reduction of adhesion, friction or wear of surface coated by these proteins is related their molecular structure. Namely, mucins are very rich in hydrophilic side-chain sugars whereas mussels foot proteins contain an uncommon type of aminoacid modification (DOPA). Such study requires considering the complex simultaneous interactions of proteins with the surfaces and neighboring proteins, as well as water and ions, which determine the surface conformation and density (coverage) of adsorbed proteins, ultimately leading to the surface properties observed at the macroscopic scale. SFA force measurements are particularly suited for this purpose because working at the nanoscale allows a better control of the surface contact geometry and a clearer distinction between adhesion, elasto-hydrodynamic vs. boundary friction and roughness effects, which are difficult to disentangle in macroscale experiments.



## A PUBLICATIONS ON SCIENTIFIC JOURNALS

## A.1 Publications on international journals

## A.1.1 Publications on international journals printed in 2012

- De Sio L., Cunningham A., Verrina V., Tone C. M., Caputo R., Bürgi T., Umeton C.P., Double active control of the plasmonic resonance of a gold nanoparticle array, Nanoscale, 2012, Vol. 4, n. 24, pp. 7619-7623.
- De Sio L., Romito M., Giocondo M., Vasdekis A., De Luca A., Umeton C.P., *Electro-switchable polydimethyl siloxane-based optofluidics*, Lab on a Chip, 2012, pp. 3760-3765.
- De Sio L., Veltri A., Caputo R., De Luca A., Strangi G., Bartolino R., Umeton C.P., Soft matter structures: from switchable diffraction gratings to active plasmonics Rivista del Nuovo Cimento, 2012, pp. 575-606.
- 4) Pezzi L., De Luca A., Veltri A., Umeton C.P., Light propagation, discrete diffraction, discrete solitons and discrete beats in periodic and non-periodic POLICRYPS structures, Nonlinear Optics Quantum Optics, 2012, pp. 269-279.
- Fasanella A., Castriota M., Cazzanelli E., De Sio L., Caputo R., Umeton C.P., Molecular orientation of E7 liquid crystal in POLICRYPS holographic gratings: a micro-Raman spectroscopic analysis, Mol. Cryst. Liq. Cryst., 2012, Vol. 558, pp. 46-53.
- Infusino M., Ferraro A., De Luca A., Caputo R., Umeton C.P., *POLICRYPS Visible Curing for Spatial Light Modulator Based Holography*, Journal of Optical Society of America B, 2012, pp. 3170-3176.
- Infusino M., De Luca A., Barna V., Caputo R., Umeton C. P., Periodic and aperiodic liquid crystal-polymer composite structures realized via spatial light modulator direct holography Optics Express, 2012, pp. 23138-23143.
- De Sio L., Ricciardi L., Serak S., La Deda M., Tabiryan N., Umeton C.P., *Photo-sensitive liquid crystals for optically controlled diffraction gratings*, Journal of materials chemistry, 2012, Vol. 22, pp. 6669-6673.
- U. Cataldi, P. Cerminara, L. De Sio, R. Caputo and C. Umeton, Fabrication and Characterization of Stretchable PDMS Structures doped with Au Nanoparticles, Mol. Cryst. Liq. Cryst. 558, 1, 22 (2012)
- R. Caputo, L. De Sio, J. Dintinger, H. Sellame, T. Scharf and C. Umeton, *Realization and Characterization of POLICRYPS-like Structures including Metallic Subentities*, Mol. Cryst. Liq. Cryst. 553, 1, 111 (2012)
- R. Caputo, L. De Sio, U. Cataldi and C. Umeton, *Plasmon resonance tunability of Gold nanoparticles embedded in a confined Cholesteric Liquid Crystal host*, Mol. Cryst. Liq. Cryst. 559, 1, 194 (2012)
- M. Ruths and B. Zappone, Direct nanomechanical measurement of an anchoring transition in a nematic liquid crystal subject to hybrid anchoring conditions, Langmuir 28 (2012) 8371-8383.
- 13) L. Marino, E. Bruno, M. P. De Santo, F. Ciuchi, S. Marino and N. Scaramuzza, Dielectric characterisation of an orthoconic antiferroelectric liquid crystal mixture,

Mol. Cryst. Liq. Cryst. 558, 120-126, (2012)

- 14) Tone CM., Pirillo S., Pucci D., De Santo MP., Barberi RC. Ciuchi F., *AFM Study of self assembled surface*, Mol. Cryst. Liq. Cryst. 558, 194-203, (2012)
- 15) F.Ciuchi, A.Mazzulla, N.Scaramuzza, E.K.Lenzi and L.R.Evangelista, Fractional diffusion equation and the electrical impedence: Experimental evidence in liquid-crystalline cells, J. Phys. Chem.C 116, 8773-8777 (2012)
- 16) M. G. Buonomenna, G. Golemme, C. M. Tone, M. P. De Santo, F. Ciuchi, E. Perrotta,, Nanostructured poly(styrene-b-butadiene-b-styrene) (SBS) membranes for the separation of nitrogen from natural gas, Adv. Funct. Mat., 22, 1759-1767, (2012)
- 17) C.M. Tone, M.P. De Santo, M.G. Buonomenna, G.Golemme and F.Ciuchi, Dynamical homeotropic and planar alignment of chromonic liquid crystals, Soft Matter, 8 (32), pp. 8478-8482, (2012)
- 18) J. L de Paula, P. A. Santoro, R. S. Zola, E. K. Lenzi, L. R. Evangelista, F. Ciuchi, A. Mazzulla, and N. Scaramuzza, Non-Debye relaxation in the dielectric response of nematic liquid crystals: Surface and memory effects in the adsorption-desorption process of ionic impurities, Phys. Rev. E, 86, 051705 (2012)
- 19) A. De Luca, M. Ferrie, S. Ravaine, M. La Deda, M. Infusino, A. R. Rashed, A. Veltri, A. Aradian, N. Scaramuzza and G. Strangi, *Gain functionalized core-shell nanoparticles: the way to selectively compensate absorptive losses*, Journal of Materials Chemistry, 22, 8846 - 8852 (2012)
- 20) L. Odorizzi, C. Ress, C. Collini, E. Morganti, L. Lorenzelli, N. Coppedè, A.B. Alabi, S. Iannotta, E. Cazzanelli, L. Vidalino and P. Macchi,
   An integrated platform for in vitro single-site cell electroporation: Controlled delivery and electrodes functionalization,
   Sensors and Actuators 170, 182-188 (2012)
- 21) 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*, Journal of Raman Spectroscopy, 43 (11), 1694-1698 (2012)
- A. Sanson, M. Giarola, B. Rossi, G. Mariotto, E. Cazzanelli, A. Speghini, *Vibrational dynamics of single-crystal YVO4 studied by polarized micro-Raman spectroscopy and ab initio calculations*, Phys. Rev. B 86 (21), 214305 (2012).
- 23) Mazzulla A, Petriashvili G, Matranga M, De Santo MP, Barberi R., *Thermal and electrical laser tuning in liquid crystal blue phase I*, Soft Matter 8, 4882-4885 (2012)
- 24) L. Marino, A.Th. Ionescu, S. Marino, N. Scaramuzza, Dielectric investigations on a bent-core liquid crystal, Journal of Applied Physics 112, 114113 (2012)
- 25) Y.G. Marinov, G.B. Hadjichristov, S. Marino, L. Todorova, S. D'Elia, C. Versace, N. Scaramuzza, A.G. Petrov, *Flexoelectro-Optical Behaviour of Layers Formed by Polymer-Liquid Crystal Phase-Separated Composites*, Bulg. J. Phys. 39 92–99 (2012)

- 26) Ruiz U., Provenzano C., Pagliusi P. Cipparrone G., Single-step polarization holographic method for programmable microlens arrays, Optics letters, vol. 37, 4958-4960 (2012).
- 27) Ruiz U., Provenzano C., Pagliusi P. Cipparrone G., Pure two-dimensional polarization patterns for holographic recording, Optics letters, vol. 37, p. 311-313(2012).
- 28) Hernandez J, Provenzano C, Pagliusi P, Cipparrone G, Optical manipulation of liquid crystal droplets through holographic polarized tweezers: Magnus effect, Molecular crystals and liquid crystals 558, 72-83, (2012).
- 29) Lepera E, Provenzano C, Pagliusi P, Cipparrone G, Liquid crystal based polarization gratings for spectro-polarimetric applications, Molecular crystals and liquid crystals 558, 109-119 (2012).
- Ruiz U, Volke Sepulveda K, Provenzano C, Pagliusi P, Cipparrone G, Generation of complex beams by means of polarization holograms, Proceedings of SPIE, The International Society for Optical Engineering, vol. 8429, 8429N. (2012).
- 31) Ruiz U, Pagliusi P, Provenzano C, Shibaev VP, Cipparrone G, Supramolecular chiral structures: Smart polymer organization guided by 2d polarization light patterns, Advanced Functional Materials, vol. 22, p. 2964 -2970(2012)

## **B** INVITED PRESENTATIONS

### **B.1** Invited presentations at international conferences in 2012

- R. Caputo, L. De Sio, C. Umeton, *Realization and characterization of light sculptured structures including liquid crystals and doped with metal nanoparticles*, Asia Communications and Photonics Conference (ACP2012), Guangzhou, China
- C. Umeton, L. De Sio, R. Caputo, U. Cataldi, L. Pezzi, *All optical switchable diffraction gratings realized in liquid crystalline composite structure with metamaterial applications*, 8th EOS Topical Meeting on Diffractive Optics (DO 2012), Delft, Netherlands
- F. Ciuchi, C.M. Tone, M.P. De Santo, M.G. Buonomenna, G. Golemme, *Alignment of chromonic liquid crystals, a difficult task,* Ist Italian-Brazilian workshop on Liquid Crystals E:Majorana Centre for Scientific culture, Erice 26-30 August 2012
- A. Mazzulla, G. Cipparrone, R.J. Hernandez, R. Bartolino, Self-organised chiral microspheres, 1st Italian-Brazilian Workshop on Liquid Crystals, Erice (Italy) 26-30 August 2012

### C PRESENTATIONS AT CONFERENCES

### C.1 Presentations at international conferences in 2012

 U. Cataldi, L. De Sio, R. Caputo, and C. Umeton, Soft matter and hard matter: a new route towards the active plasmonics, 10th Conference of the Italian Society of Liquid Crystals (SICL), Rome, Italy (2012)

## 2) A. De Luca,

Bringing Gain to Metamaterials: a Way to Selectively Compensate Absorptive Losses, International Conference on Metamaterials and Dissemination Workshop 2012, Jena (Germany)

- A. De Luca *Routing Light with Spatial Solitons: Light Localization and Steering in Liquid Crystals,* Case Western Reserve University – Condensed Matter Seminar (February 2012), Cleveland (OH – USA)
- De Luca, Bringing Gain to Metamaterials: a Way to Selectively Compensate Absorptive Losses, CNR – IPCF Messina, Lab Visit and Seminar (June 2012)
- E. Cazzanelli, G. Chiarello, T. Caruso, M. Castriota, A. Politano, M. Giarola and G. Mariotto, Growth and characterization of graphene layers deposited on Pt (111) surface, "E-MRS 2012 SPRING MEETING" Congress Center - 14/05 – 18/05/2012, Strasbourg, France.
- E. Cazzanelli, G. Chiarello, T. Caruso, M. Castriota, A. Politano, M. Giarola and G. Mariotto, *Crescita via CVD e caratterizzazione di grafene su Pt (111)*". GISR-II CONGRESSO NAZIONALE di SPETTROSCOPIE RAMAN ed EFFETTI OTTICI NON LINEARI", 06/06 – 08/06/2012 Bologna, Italy
- 7) Cipparrone G, Hernandez RJ, Mazzulla A et al., *Chiral Self-assembled Solid Microspheres*, 13th International Symposium on Colloidal and Molecular Electrooptics, ELOPTO 2012, September, 2012 Gent (Belgium)
- Cipparrone G, Mazzulla A, Hernandez RJ et al., *Chiral Self-assembled Solid Microspheres: optical control and photonics applications*, Istitute for Chemical-Physical Processes - General Meeting 2012 - 21-23 May 2012, Cetraro (CS), Italy
- L. Marino, E. Bruno, S. Marino, A. Th. Ionescu, N. Scaramuzza Dielectric characterisation of gold nanoparticles/antiferroelectric liquid crystal composites, Broadband Dielectric Spectroscopy (BDS) and its Application, 03-09 September 2012, Lipsia (Germany)
- Ruiz. U, Volke-Sepulveda K., Provenzano C., Pagliusi P., Cippparrone G., Generation of complex beams by means of polarization holograms, SPIE Photonics Europe, 16-19/04/2012, Bruxelles, Belgium
- G. Cipparrone, J.R. Hernandez, Volke-Sepulveda K. et al., *Chiral Self-assembled Solid Microspheres: optical control and photonics applications*, IPCF (Istituto per i Processi Chimico-Fisici) Meeting, 21-23/05/2012, Cetraro(CS), Italy
- Hernandez J.R., Provenzano C., Pagliusi P., Cippparrone G., *The Magnus force effect in optical micromanipulation*, IPCF (Istituto per i Processi Chimico-Fisici) Meeting, 21-23/05/2012, Cetraro (CS), Italy
- G. Cipparrone, J.R. Hernandez, et al., *Chiral Self-assembled Solid Microspheres*, 13th International Symposium on Colloidal and Molecular Electrooptics, 2-5/9/2012, Gent, Belgium
- R. Hernandez, P. Pagliusi, C. Provenzano, G. Cipparrone, *The Magnus force effect in optical micromanipulation*, 13th International Symposium on Colloidal and Molecular Electrooptics, 2-5/9/2012, Gent, Belgium.

## OTHER PRESENTATIONS AND EVENTS

The research project of the spin-off enterprise NOTREDAME, generated by the university research group, after two evauation processes, has been admitted in the strategic agenda of the "Polo delle Innovazioni dei Materiali e della Produzione" supported by the Region Calabria.

Interview with "LE SCIENZE" (Italian edition of Scientific American): pp. 16-17, N°526, June 04, 2012 about the
technological transfer project NOTREDAME.

Interview with "PANORAMA" (Italian weekly magazine): p. 139, November 28, 2012 about the technological transfer project NOTREDAME.

Admission of the project NOTREDAME to the final rush of the ENEL-LAB competition.

COST Action MP1205, ADVANCES IN OPTOFLUIDICS: INTEGRATION OF OPTICAL CONTROL AND PHOTONICS WITH MICROFLUIDICS, Chair Gabriella Cipparrone.

Progetto di Grande Rilevanza Italia-Messico 2011-2013: Strategie di manipolazione ottica della materia soffice mediante pinze olografiche con gradiente di polarizzazione.

**Metachem European Project:** University of Vigo (Vigo, Spain), CNRS - Centre National de Recherche Scientifique (Bordeaux – Paris, France)), CNR-IPCF (UOS Cosenza – UOS Bari, Italy), University of Manchester (UK), Helsinki University of Technology (Finland), Université Catholique de Louvain (Belgium), Università degli studi di Siena (Italy), Fraunhofer Gesellschaft zur Förderung der angewandten Forschung e. V. (Germany), Rhodia LOF (France)

Nanoplasm Lab Project: Case Western Reserve University (OH – USA)

#### PATENTS

1) Marco Castriota, Enzo Cazzanelli, Giuseppe De Santo, Massimo La Deda and Roberto Termine, "ELECTROCHROMIC DEVICE". Italian Patent Office. PTC/IT2012/000309, 08/10/2012, ROME, ITALY.

#### 8. SURFACE ELECTRON SPECTROSCOPY (SPES)

Professors and				
Researchers	Elio Colavita			
	Gennaro Chiarello			
	Raffaele Giuseppe Agostino			
	Vincenzo Formoso			
	Tommaso Caruso			
Postdoc fellows	Alfonso Policicchio			
	Antonio Politano			
PhD students	Marco Caputo			
Technicians	Salvatore Abate (Lycril/CNR)			
	Giovanni Desiderio (Lycril/CNR)			
	Vito Fabio			
	Eugenio Li Preti			
Collaborators	G. Benedek (Università Milano-Bicocca, Italy)			
	D. Farías (Universidad Autonoma de Madrid, Spain)			
	R. Miranda (IMDEA Nanociencia, Madrid, Spain)			
	F. de Juan (Berkeley National Laboratory, Usa)			
	V. Alzari (University of Sassari, Italy)			
	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. Nagy (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, Catania, 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)			

#### Research subjects:

- 8.1 GRAPHENE/METAL INTERFACES
  - 8.1.1 Dispersion and Damping Processes of  $\pi$  Plasmon in Monolayer Graphene on Pt(111)
  - 8.1.2 Evidence of Kohn anomalies in quasi-freestanding graphene on Pt(111)
  - 8.1.3 Phonon dispersion of quasi-freestanding graphene on Pt(111)
  - 8.1.4 Effects of a humid environment on the sheet plasmon resonance in epitaxial graphene
  - 8.1.5 Elastic properties of a macroscopic graphene sample from phonon dispersion measurements.

<sup>8.2</sup> SPECTROSCOPIC AND MICROSCOPIC STUDIES OF CARBON AND METAL-OXIDE NANOSTRUCURES. 8.21 ZnTPP dye adsorption on nanostructured TiO<sub>2</sub>.

#### Introduction

The activity of the Group is driven by the MaTeRia project. This is an highly specialized laboratory organized in three progressive levels.

In the First level, STAR (Southern Europe Thomson Back-Scattering Source for Applied Research) equipped with the beam-line  $\mu$ Tomo, will be built This laboratory consists in an advanced X-ray source, based on the Thomson Back-Scattering,;

the second level will be equipped with some laboratories:

- 1. Preparation and characterization
- 2. Characterization of the mechanical and physical properties
- 3. Modeling and simulation
- 4. Prototyping
- 5. Advanced spectroscopy;

the third level. will be the network of existent departmental laboratories .

#### MaTeRiA/STAR SITE at UniCal



#### 8.1 GRAPHENE/METAL INTERFACES

#### 8.1.1 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.

#### 8.1.2 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<sub>2g</sub> and K-A<sub>1</sub>' 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.

#### 8.1.3 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).

#### 8.1.4 Effects of a humid environment on the sheet plasmon resonance in epitaxial graphene

High-resolution electron energy loss spectroscopy has been used to study the influence of a humid environment on the collective electronic excitations of a quasi-freestanding graphene monolayer supported on Pt(111). We found that the adsorption of water molecules at room temperature on graphene/Pt(111) is dissociative and it gives rise to adsorbate fragments. Our results indicate that these adsorbed species change the energy, the dispersion, and the lifetime of the graphene sheet plasmon. Moreover, the phase velocity of this low-energy collective mode decreases by 11% even if its lifetime notably increases. By contrast, humidity has a negligible effect on the energy of the  $\pi$  plasmon at 6 eV and the unique effect induced by humidity is a significant attenuation of its intensity. Such information is essential for tailoring graphene-based plasmonic devices which should operate in ambient air humidity

#### 8.1.5 Elastic properties of a macroscopic graphene sample from phonon dispersion measurements

The average elastic properties and the interatomic force constants of a quasi-freestanding graphene sample have been evaluated by analyzing the phonon dispersion measured by means of angle-resolved energy loss spectroscopy. We found a Poisson's ratio of 0.19 and a Young's modulus of 342 N/m. Such findings are in excellent agreement with calculations performed for a free-standing graphene membrane. Present results indicate that the high crystalline quality of graphene grown on metal substrates leads to macroscopic samples of high tensile strength and bending flexibility to be used for technological applications such as electromechanical devices and carbon-fiber reinforcements

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

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

This research activity is still in progress.

In the field of dye sensitized solar cells (DSSC), based on a nanostructured TiO2 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 TiO2 surface is still under investigation. In order to elucidate the formation mechanisms and the properties of the TiO2-dye molecule interface, photoelectron spectroscopies have been employed exploiting their high surface sensitivity. However, most of the work has been carried out on TiO2 single crystals, while in a standard DSSC, the TiO2 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  $TiO_2$  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  $TiO_2$  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  $TiO_2$  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, and charge transfer between phenyl rings and substrate is quenched when a Zn-TPP monolayer is grown on pristine and fully oxidized  $TiO_2$  films.

#### A PUBLICATIONS ON SCIENTIFIC JOURNALS

#### A.1 Publications on international journals in 2012

- Politano A., Marino A. R., Formoso V., Chiarello G. Evidence of Kohn anomalies in quasi-freestanding graphene on Pt(111) Carbon, Vol. 50, 734-736 (2012)
- Politano, A., Marino, A.R., Chiarello, G. *Effects of a humid environment on the sheet plasmon resonance in epitaxial graphene* Physical Review B, Vol. 86, 085420 (2012)
- Politano A., Marino A. R., Formoso V., Chiarello G. *Phonon dispersion of quasi-freestanding graphene on Pt(111)* Journal of Physics: Condensed Matter, Vol. 24, 104025 (2012)
- Politano A., Marino A. R., Formoso V., Farías D., Miranda M., Chiarello G. *Quadratic dispersion and damping processes of π plasmon in monolayer graphene on Pt(111)* Plasmonics, Vol. 7, 369-376 (2012)
- Politano A., Marino A. R., Campi D., Farías D., Miranda M., Chiarello G. *Elastic properties of a macroscopic graphene sample from phonon dispersion measurements* Carbon, Vol. 50, 4903-4910 (2012)
- Díaz C., Fernández Cuñado J. L., Politano A., Maccariello D., Martín F., Farías D., Miranda R. *He, Ne and Ar scattering from Ru(0001)* Journal of Physics: Condensed Matter, Vol. 24, 354002 (2012)
- Caputo M., Di Santo G., Parisse P., Petaccia L., Floreano L., Verdini A., Panighel M., Struzzi C., Taleatu B., Lal C., Goldoni M. Experimental Study of Pristine and Alkali Metal Doped Picene Layers: Confirmation of the Insulating Phase in Multilayer Doped Compounds

Journal of Physical Chemistry C, Vol. 116, 19902–19908 (2012)

#### A.2 Book chapters

 Politano, A., Chiarello G. *Influence of electron quantum confinement on the electronic response of metal/metal interfaces* Reviews in Plasmonics, Springer Ed. C.D. Geddes pp 69-104 (2012).

#### INTERNATIONAL AND NATIONAL PROJECTS

- Project full title: Membrane nanocomposite avanzate ed elettrocatalizzatori innovativi per celle a combustibile ad elettrolita polimerico a lunga durata, NAMED-PEM Italian PRIN 2010-2011 project Name of the coordinating person: Dr. S. Panero (Roma-La Sapienza)Funded in 2012
- 2. Project MaTeRiA (materials, technologies and advanced research) Uso della radiazione X da retrodiffusione Thomson emessa dalla sorgente STAR

#### 9. THEORETICAL PARTICLE PHYSICS AND APPLICATIONS

Professors and Researchers	Roberto Fiore Domenico Giuliano Alessandro Papa Marco Rossi
Postdoc fellows	Francesco Caporale Gabriele Infusino
PhD students	Giacinto Ciappetta ( <i>XXV cycle</i> ) Beatrice Murdaca ( <i>XXV cycle</i> ) Amedeo Perri ( <i>XXVI cycle</i> )
Collaborators	<ul> <li>I. Affleck (University of British Columbia, Vancouver, Canada)</li> <li>O. Borisenko (Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine)</li> <li>A. Brunetti (Heinrich Heine Universität, Düsseldorf, Germany)</li> <li>G. Campagnano (Università "Federico II" di Napoli)</li> <li>P. Cea (Università di Bari &amp;INFN-Bari, Italy)</li> <li>V. Chelnokov (Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine)</li> <li>A. Cirillo (Università di Perugia &amp; INFN-Perugia, Italy)</li> <li>G. Cottese (Università di Caragoza, Spain)</li> <li>L. Cosmai (INFN-Bari, Italy)</li> <li>M. D'Elia (Università di Genova &amp; INFN-Genova, Italy)</li> <li>V.S. Fadin (Budker Institute for Nuclear Physics, Novosibirsk, Russia)</li> <li>S. Fazio (Brookhaven National Laboratory)</li> <li>D. Fioravanti (Università di Bologna &amp; INFN-Bologna, Italy)</li> <li>P. Giudice (University of Swansea)</li> <li>A.V. Grabovsky (Budker Institute for Nuclear Physics, Novosibirsk, Russia)</li> <li>M. Gravina (University of Cyprus)</li> <li>P. Grinza (University of Cyprus)</li> <li>P. Grinza (University of Cyprus)</li> <li>P. Grinza (Università della Calabria, Italy)</li> <li>N. Lu Ivanov (Sobolev Isntitute for Theoretical Physics, Kiev, Ukraine)</li> <li>A. Lavorini (Università della Calabria, Italy)</li> <li>P. Lucignano (CNR Napoli)</li> <li>V. Magas (Università della Calabria, Italy)</li> <li>F. Plastina (Università della Calabria, Eury)</li> <li>F. Sanfilippo (Università della Calabria &amp; INFN-Perugia, Italy)</li> <li>F. Sanfilippo (Università della Calabria &amp; INFN-Cosenza)</li> <li>D. Rossini (Scuola Normale Superiore, Pisa, Italy)</li> <li>F. Sanfilippo (Università della Calabria &amp; INFN-Cosenza)</li> <li>P. Sodano (Università della Calabria &amp; INFN-Cosenza)</li> <li>P. Sodano (Università della Calabria &amp; INFN-Perugia, Italy &amp; International Institute of Physics, Natal, Brasil)</li> <li>I. Surzhikov (Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine)</li> <li>A. Trombettoni (SISSA-Trieste, Italy)</li> <li>V.R. Zoller (ITEP, Mosco</li></ul>

#### Introduction

The research activity during the AA 2011-12 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 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 was proven and a method of restoration was worked out. The operators for articolar from the standard BFKL kernel to the quasi-conformal one were found both in Möbius and total representations.

As it was recently shown, the colour singlet BFKL kernel, taken in Möbius representation in the space of impact parameters, can be written in quasi-conformal shape, which is unbelievably simple compared with the conventional artico the BFKL kernel in momentum space. It was also proved that the total kernel is completely defined by its Möbius representation. We calculated the difference between standard and quasi-conformal BFKL kernels in momentum space and discovered that it is rather simple. Therefore we came to the conclusion that the simplicity of the quasi-conformal kernel is caused mainly by using the impact parameter space.

We recalculated, completely within the original BFKL approach and at the next-to-leading order, the jet vertex relevant for the production of Mueller-Navelet jets in proton collisions and of forward jets in DIS. We considered both processes with incoming quark and gluon. The starting point was the definition of quark and gluon impact factors in the BFKL approach. Following this procedure we showed explicitly that all infrared divergences cancel when renormalized parton densities are considered. We compared our results for the vertex with the former calculation of Bartels *et al.* And, in the case of the quark contribution, clarified the discrepancy present in the literature.

We considered within QCD collinear factorization the process proton-proton to jet + jet +X, where two forward high $p_T$  jets are produced with a large separation in rapidity (Mueller-Navelet jets). In this case the (calculable) hard part of the reaction receives large higher-order corrections, which can be accounted for in the BFKL approach. In articolar, we calculated in the next-to-leading order the impact factor (vertex) for the production of a forward high- $p_T$ , in the approximation of small aperture of the jet cone in the pseudorapidity-azimuthal angle plane. The final expression for the vertex turned out to be simple and easy to implement in numerical calculations.

We considered within QCD collinear factorization the inclusive process proton-proton to  $h_1 + h_2 + X$ , where the pair of identified hadrons ( $h_1$ ,  $h_2$ ) having large transverse momenta is produced in high-energy proton-proton collisions. In

articolar, we concentrated on the kinematics where the two identified hadrons in the final state are separated by a large interval of rapidity. In this case the (calculable) hard part of the reaction receives large higher order corrections. We provided a theoretical input for the resummation of such contributions with next-to-leading logarithmic accuracy (NLA) in the BFKL approach. Specifically, we calculated in NLA the vertex (impact-factor) for the inclusive production of the identified hadron. This process has much in common with the widely discussed Mueller-Navelet jets production and can be also used to access the BFKL dynamics at proton colliders.

#### 9.1.2 Hadron Phenomenology

We discussed heavy quark contributions to the neutrino-nucleon total cross section at very high energies, well above the real top production threshold. The top-bottom weak current is found to generate strong left-right asymmetry of neutrinonucleon interactions. We separated contributions of different helicity states and made use of the  $k_t$ -factorization to derive simple and practically useful formulas for the left-handed ( $F_L$ ) and right-handed ( $F_R$ ) components of the conventional structure function  $2xF_3 = F_{L-}F_R$  in terms of the integrated gluon density. We showed that  $F_L$  is much larger that  $F_R$  and,

consequently,  $xF_3$  is similar to  $F_T$ , where  $F_T$  is the transverse structure function. The conventional structure function  $F_2=F_s+F_T$  at  $Q^2$  much smaller than the squared top mass appears to be dominated by its scalar (also known as longitudinal) component  $F_S$  and the hierarchy  $F_S \gg F_L \gg F_R$  arises naturally. We evaluated the total neutrino-nucleon cross section at ultrahigh energies within the color dipole BFKL formalism.

Exclusive diffractive production of real photons and vector mesons in ep 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.

We showed how the familiar phenomenological way of combining the  $Q^2$  (photon virtuality) and t (squared momentum transfer) dependences of the scattering amplitude in Deeply virtual Compton Scattering (DVCS) and Vector Meson

Production (VMP) processes can be understood in an off-mass-shell generalization of dual amplitudes with Mandelstam analyticity. By comparing different approaches, we managed also to constrain the numerical values of the free parameters.

#### 9.2 LATTICE GAUGE THEORIES

#### 9.2.1 Finite density QCD

We determined the (pseudo)critical lines of QCD with two degenerate staggered fermions at nonzero temperature and quark or isospin density, in the region of imaginary chemical potentials; analytic continuation was then used to prolongate to the region of real chemical potentials. We obtained an accurate determination of the curvatures at zero chemical potential, quantifying the deviation between the case of finite quark and of finite isospin chemical potential. Deviations from a quadratic dependence of the pseudocritical lines on the chemical potential were clearly seen in both cases: we tried different extrapolations and, for the case of nonzero isospin chemical potential, confronted them with the results of direct Monte Carlo simulations. Finally we found that, as for the finite quark density case, an imaginary isospin chemical potential can strengthen the transition until turning it into strong first order.

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

#### 9.2.2 Confinement in QCD

We analyzed the transverse profile of the chromoelectric flux tubes in SU(2) and SU(3) pure gauge theories by a simple variational ansatz, using a strict analogy with ordinary superconductivity. Our method allowed to extract the penetration length and the coherence length of the flux tube.

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

We investigated both analytically and numerically the renormalization group equations in two-dimensional (2D) Z(N) vector models. The position of the critical points of the two phase transitions for N > 4 was established and the critical index \nu was computed. For N = 7 and 17 the critical points were located by Monte Carlo simulations and some of the corresponding critical indices were determined. The behavior of the helicity modulus was studied for N = 5, 7, and 17. Using these and other available Monte Carlo data we discussed the scaling of the critical points with N and some other open theoretical problems.

We performed an analytical and numerical study of the phase transitions in three-dimensional Z(N) lattice gauge theories at finite temperature for N > 4, exploiting the equivalence of these models with a generalized version of the two-dimensional vector Potts models in the limit of vanishing spatial coupling. In this limit the Polyakov loops play the role of



Z(N) spins. The effective couplings of these two-dimensional spin models were calculated explicitly. It was argued that the effective spin models have two phase transitions of BKT type. This was confirmed by large-scale Monte Carlo simulations. Using a cluster algorithm we located the position of the critical points and studied the critical behavior across both phase transitions in detail. In particular, we determined various critical indices and computed the helicity modulus, the average action, and the specific heat. A scaling formula for the critical points with N was proposed.

#### 9.2.4 Planar QED in external fields

We investigated planar quantum electrodynamics with two degenerate staggered fermions in an external magnetic field on the lattice. We argued that in external magnetic fields there is dynamical generation of mass for two-dimensional massless Dirac fermions in the weak-coupling region. We extrapolated our lattice results to the quantum Hall effect in graphene.

#### 9.3 FIELD THEORY OF CORRELATED DEVICES

### 9.3.1 Junctions of interacting quantum wires and mathematical model for SNS junctions made with topological superconductors

Using a similarity Hamiltonian renormalization procedure, we determine an effective spin-1/2 representation of the Bose-Hubbard model at halfinteger filling and at a finite on-site interaction energy U. By means of bosonization, we traded the effective Hamiltonian as that of a spin-1/2 XXZ magnetic chain with renormalized coupling and anisotropy parameters. Going through this mapping, we provide analytical estimates of the correlation functions of the Bose-Hubbard model and compare the analytical results with those based on DMRG numerical simulations. We find an excellent agreement up to 10% between the output of analytical and numerical computations, even for relatively small values of U. Our analysis implies that, also at finite U, the 1D Bose-Hubbard model with suitably chosen parameters may be seen as a quantum simulator of the XXZ chain.



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 Spin-chain representation of the lattice Bose-Hubbard chain

We showed that, in the limit of a long junction, the dc Josephson current through a long SNS junction, which typically receives contributions from both Andreev bound states localized in the normal region as well as from scattering states incoming from the superconducting leads, at low temperatures, can be expressed entirely in terms of properties of the Andreev bound states at the Fermi energy: the normal and Andreev reflection amplitudes at the left-hand and at the right-hand S-N interface. Our final result is a "Landauer-like" formula for the Josephson current across a long junction. Moreover, our derivation has important implications for treating interactions, as well as nonequilibrum, in such systems. Moreover, we have investigated the applicability of the fermionic renormalization group approach developed by Matveev and Glazman to a junction of interacting quantum wire. While, on one hand, we have been able to recover previous results on a Y-junction of three quantum wires derived within Luttinger liquid framework, we are now planning to extend the fermionic approach to systems that typically cannot be dealt with within Luttinger liquid approach, except perturbatively, such as, for instance, junctions involving superconductors and interacting quantum wires.

#### 9.3.3 Topogical Kondo effect due to emerging Majorana modes in Josephson junction networks

We have derived the phase diagram of a junction made with K interacting quantum wires connected to a topological superconductor with a localized Majorana fermion at the interface. We showed that a novel phase emerges in such a phase diagram, corresponding to a finite-coupling fixed point. The corresponding fixed point has been investigated and characterized by deriving both at the dc conductance tensor of the junction and at the boundary entropy of the system. In particular, the results concerning the boundary entropy at the fixed points of the phase diagram appear to be in perfect agreement with Affleck-Ludwig's "g theorem" for boundary interaction Hamiltonians. The results are contained in a paper in preparation.

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

In collaboration with D. Fioravanti, M. Rossi completed a first project concerning twist operators in the sl(2) sector of planar N=4 SYM in a special limit in which the relevant dynamics should be give by integral equations of the O(6) nonlinear 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 all loops result.

A second project, collaboration between D. Fioravanti, G. Infusino and M. Rossi, concerns the study of reciprocity and

functional relations in anomalous dimensions of twist operators in N=4 SYM. In particular we performed precision computations of corrections to the anomalous dimension going like the inverse power of the Lorentz spin.

Other three projects are in progress. The first concerns the study of excitations on the GKP vacuum. In particular we are interested in determining scattering phases between excitations and dispersion relations of the latters. This project is carried on by M.Rossi in collaboration with D. Fioravanti and his PhD student S. Piscaglia.

The second project is aimed at studying a set of TBA equations with boundary. Following the seminal paper of Correa, Maldacena, Sever this set of integral equations can be used to determine by means of the AdS/CFT correspondence the potential between coloured particles in a supersymmetric theory. This project is carried on by M. Rossi in collaboration with D. Bombardelli and D. Fioravanti. The third project involves G. Infusino and concerns numerical solutions of sl(n) Bethe equations.

#### A PUBLICATIONS ON SCIENTIFIC JOURNALS

#### A.1 Publications on international journals

#### A.1.1 Publications on international journals printed in 2012

- V.S. Fadin, R. Fiore, A.V. Grabovsky and A. Papa, *Connection between complete and Möbius forms of gauge invariant operators*, Nucl. Phys. B 856 (2012) 111-124.
- V.S. Fadin, R. Fiore and A. Papa, Difference between standard and quasi-conformal BFKL kernels, Nucl. Phys. B 865 (2012) 67-82.
- F. Caporale, D.Yu. Ivanov, B. Murdaca, A. Papa and A. Perri, *The next-to-leading order jet vertex for Mueller-Navelet and forward jets revisited*, JHEP02(2012)101, 27 pages.
- D.Yu. Ivanov and A. Papa, *The next-to-leading order forward jet vertex in the small-cone approximatio*", JHEP05(2012)086, 31 pages.
- D.Yu. Ivanov and A. Papa, Inclusive production of a pair of hadrons separated by a large interval of rapidity in proton collisions, JHEP07(2012)045, 29 pages.
- S. Fazio, R. Fiore, L. Jenkovszky, A. Lavorini, Exclusive diffractive production of real photons and vector mesons in a factorized Regge-pole model with non-linear Pomeron trajectory, Phys. Rev. D85 (2012) 054009
- R. Fiore, V.R. Zoller, Heavy quark currents in ultra-high energy neutrino interactions, JETP Lett. 95 (2012) 55-60
- R. Fiore, L.L. Jenkovszky, A. Lavorini, V.K. Magas, On the interplay between Q<sup>2</sup> and t dependences in exclusive diffractive production of real photons and vector mesons in ep collisions, Ukr. J. Phys. 57 (2012) 1197
- P. Cea, L. Cosmai, M. D'Elia, A. Papa, F. Sanfilippo, *The critical line of two-flavor QCD at finite isospin or baryon densities from imaginary chemical potentials*, Phys. Rev. D 85 (2012) 094512, 11 pages.
- P. Cea, L. Cosmai and A. Papa, *Chromoelectric flux tubes and coherence length in QCD*, Phys. Rev. D 86 (2012) 054501, 10 pages.
- O. Borisenko, V. Chelnokov, G. Cortese, R. Fiore, M. Gravina and A. Papa, *Phase transitions in two-dimensional Z(N) vector models for N>4*, Phys. Rev. E 85 (2012) 021114, 9 pages.
- O. Borisenko, V. Chelnokov, G. Cortese, R. Fiore, M. Gravina, A. Papa and I. Surzhikov, *Phase transitions in strongly coupled 3d Z(N) lattice gauge theories at finite temperature*, Phys. Rev. E 86 (2012) 051131, 14 pages.
- P. Cea, L. Cosmai, P. Giudice and A. Papa, *Chiral Symmetry Breaking in Planar QED in External Magnetic Fields*, Phys. Rev. D 85 (2012) 094505, 6 pages.

14. D. Fioravanti and M. Rossi, TBA-like equations and Casimir effect in (non-)perturbative AdS/CFT, JHEP12(2012)013

#### B PUBLICATIONS ON CONFERENCE PROCEEDINGS B.1 Publications on international conference proceedings in 2012

- P. Cea, L. Cosmai, M. D'Elia, A. Papa and F. Sanfilippo, *Two-flavor QCD at finite quark or isospin density*, Proceedings of the 30th International Symposium on Lattice Gauge Theories, June 24 - 29, 2012, Cairns, Australia; editors D. Leinweber et al., PoS(Lattice 2012)067, [arXiv:1212.5896].
- O. Borisenko, V. Chelnokov, G. Cortese, R. Fiore, M. Gravina, A. Papa, I. Surzhikov, *BKT phase transitions in strongly coupled 3D Z(N) LGT at finite temperature*, Proceedings of the 30th International Symposium on Lattice Gauge Theories, June 24 - 29, 2012, Cairns, Australia; editors D. Leinweber et al., PoS(Lattice 2012)270. [arXiv:1212.1051].

#### C PRESENTATIONS AT SCHOOL AND CONFERENCES

#### C.1 Presentations at international schools and conferences in 2012

- D.Yu. Ivanov and A. Papa, *The NLO jet vertex for Mueller-Navelet and forward jets in the small-cone approximation*, talk given by A. Papa at DIS 2012, Bonn, 26-30 March 2012, doi:http://indico.cern.ch/contributionDisplay.py?contribId=260&confId=153252 arXiv:1208.3293
- F. Caporale, D.Yu. Ivanov, B. Murdaca, A. Papa, A. Perri, *The jet vertex for Mueller-Navelet and forward jet production*, talk given by B. Murdaca at the 3rd Young Researchers Workshop "Physics Challenges in the LHC Era", Frascati, May 7 and 10, 2012; arXiv:1207.6183
- F. Caporale, D.Yu. Ivanov, B. Murdaca, A. Papa, *Mueller-Navelet jets in high-energy hadron collisions*, talk given by F. Caporale at "Diffraction 2012", Puerto del Carmen, 10-15 Sept. 2012, to appear in the proceedings (AIP), arXiv:1209.6233
- 4. F. Caporale, D.Yu. Ivanov, B. Murdaca, A. Papa, A. Perri, *NLO forward jet vertex*, talk given by B. Murdaca at "Diffraction 2012", Puerto del Carmen, 10-15 Sept. 2012, to appear in the proceedings (AIP), arXiv:1212.0487

# UNIVERSITÀ DELLA CALABRIA

## Dipartimento di FISICA