

**XL Congresso Nazionale di Chimica Fisica
(23-27 Giugno 2013)**

24 Giugno 2013

8.45-9.00		Cerimonia di Apertura
Sessione 1: Nano e Biomateriali		
<i>Chair:</i>		
9.00-9.45	PL1	FUNCTIONAL MATERIALS BY SELF-ASSEMBLY. PROPERTIES AND APPLICATIONS
		<i>Luisa de Cola (Univ. Strasbourg, France)</i>
9.45-10.00	1O1	MAGNETIC-PLASMONIC NANOALLOYS: A NEW CLASS OF MULTIMODAL THERANOSTIC TOOLS
		<i>V. Amendola, S. Scaramuzza, M. Meneghetti</i>
10.00-10.15	1O2	PREPARATION AND STRUCTURAL CHARACTERIZATION OF FUNCTIONALIZED THERANOSTIC NANOPARTICLES
		<i>A. Luchini, G. Mangiapia, G. Vitiello, G. d'Errico, D. Montesarchio</i>
10.15-10.30	1O3	HYDROGEL NANOPARTICLES FOR ENZYME-BASED THERAPIES
		<i>S. Bobone, E. Miele, B. Cerroni, E. Nicolai, A. di Venere, E. Placidi, G. Paradossi, N. Rosato, L. Stella</i>
10.30-10.45	1O4	FLUORESCENT MAGNETIC NANOPARTICLES AS BIOSENSORS
		<i>F. Canepa, M.A. Lucchini, P.Riani, M. Alloisio</i>
10.45-11.00	1O5	THE EFFECT OF LANTHANIDE IONS DOPANTS ON THE LUMINESCENCE PERFORMANCES OF RARE EARTH OXYCARBONATES
		<i>F. Locardi, L. Panzieri, M. Fasoli, M. Martini, I. Miletto, E. Bottinelli, E. Gianotti, C. Artini, V. Caratto, R. Masini, E. Franceschini, G.A Costa</i>
11.00-11.20		<i>Coffee-break</i>
<i>Chair:</i>		
11.20-11.45	KN1	SMART LIPIDS ASSEMBLIES FOR PROGRAMMABLE NANOMATERIALS: STRUCTURE AT THE NANOSCALE AND INTERACTION WITH MEMBRANE MODELS
		<i>D. Berti, C. Montis, M. Bonini, P. Baglioni</i>
11.45-12.00	1O6	CYCLOPEPTOIDS: VERSATILE BUILDING BLOCKS FOR NEW MATERIALS

		<i>C. Tedesco, I. Izzo, L. Erra, B. Nardone, F. De Riccardis</i>
12.00-12.15	107	SILICA-BASED MATERIALS IN PHARMACEUTICAL FORMULATIONS: AN INSIGHT FROM QUANTUM-MECHANICAL SIMULATION
		<i>M. delle Piane, M. Corno, P. Ugliengo</i>
12.15-12.30	108	MESOPOROUS SILICA NANOPARTICLES WITH TUNABLE PORE SIZE FOR TAILORED GOLD NANOPARTICLES
		<i>G. Sponchia, R. Marin, I. Freris, E. Moretti, L. Storaro, P. Canton, A. Benedetti, A. Lausi, P. Riello</i>
12.30-12.45	109	CHEMICAL-PHYSICAL PROPERTIES OF ULTRASMALL SUPERPARAMAGNETIC IRON OXIDE NANOPARTICLES WITH TITANIUM-N,N-DIALKYL CARBAMATE COATING
		<i>V. Domenici, S. Dolci, C. Duce, Z. Jaglicic, A. Boni, G. Pampaloni, M.R. Tinè</i>
12.45-13.00	1010	BLOCK COPOLYMERS LITHOGRAPHY: BOTTOM UP MEETS TOP DOWN
		<i>M. Perego, F. Ferrarese Lupi, T.J. Giammaria, G. Seguni, L. Boarino, V. Gianotti, K. Sparnacci, D. Antonioli, M. Laus</i>
13.00-14.30		<i>Pranzo a Buffet</i>

Sessione 2: Spettroscopia, Struttura e Processi Molecolari

<i>Chair:</i>		
14.30-14.55	KN2	MOLECULAR DYNAMICS AND ELECTRON SPIN RELAXATION
		<i>Marina Brustolon, A. Barbon</i>
14.55-15.10	201	DENDRIMERS FOR BIOMEDICAL APPLICATIONS CHARACTERIZED BY MEANS OF SPIN PROBES AND SPIN LABELS
		<i>M.F. Ottaviani, D. Appelhans, F.J. De la Mata, S. Garcia-Gallego, A. Fattori, C. Coppola, M. Cangiotti, S. Lucchi, J.P. Majoral, D.K. Smith, N. Garti, B. Klajnert</i>
15.10-15.25	202	UNRAVELLING ELECTRONIC AND STRUCTURAL REQUISITES OF TRIPLET-TRIPLET ENERGY TRANSFER BY ADVANCED ELECTRON PARAMAGNETIC RESONANCE
		<i>M. di Valentin, E. Salvadori, L. Orian, A. Polimeno, V. Barone, D. Carbonera</i>
15.25-15.40	203	ROTATIONAL SPECTROSCOPY MEETS THEORY: THE CHALLENGE OF BIOMOLECULES
		<i>C. Puzzarini</i>

15.40-15.55	204	STRUCTURAL AND DYNAMICAL PROPERTIES OF LOW-DENSITY AND HIGH-DENSITY LIQUID WATER
		<i>A. Lapini, S. Fanetti, M. Pagliai, M. di Donato, M. Citroni, S. Scandolo, R. Bini, R. Righini</i>
15.55-16.10	205	MODULATED EXCITATION SPECTROSCOPY: A POWERFUL TOOL TO ENHANCE SENSITIVITY OF SPECTROSCOPIC TECHNIQUES
		<i>G.L. Chiarello, D. Ferri</i>
16.10-16.30		<i>Coffee-break</i>
<i>Chair:</i>		
16.30-16.45	206	INSIGHTS INTO ADSORPTION OF NH₃ ON HKUST-1 METAL ORGANIC FRAMEWORK: A MULTITECHNIQUE APPROACH
		<i>F. Bonino, E. Boefecchia, S. Maurelli, D. Gianolio, E. Groppo, M. Chiesa, C. Lamberti</i>
16.45-17.00	207	A COMBINED APPROACH TO THE STUDY OF CEMENT HYDRATION USING X RAY POWDER DIFFRACTION AND SOLID STATE MULTINUCLEAR RESONANCE SPECTROSCOPY
		<i>F. Canonico, E. Boccaleri, G. Paul, L. Marchese, D. Gastaldi</i>
17.00-17.15	208	CONFORMATIONAL DISTRIBUTION OF BIOACTIVE MOLECULES INVESTIGATED BY NMR SPECTROSCOPY IN ORDERED MEDIA
		<i>G. De Luca, M.E. di Pietro, G. Celebre, M. Longeri</i>
17.15-17.30	209	STRONG AND WEAK HYDROGEN BONDS IN THE ISOLATED MONO-HIDRATED S-CIS AND S-TRANS ACRYLIC ACIDS
		<i>A. Maris, C. Calabrese, W. Caminati, L. Evangelisti, L. Favero, G. Feng, Q. Gou, S. Melandri</i>
17.30-17.45	2010	SURFACTANT-BASED SYSTEMS FOR THE CLEANING OF WORKS OF ART: STRUCTURE AND CLEANING MECHANISM
		<i>M. Baglioni, M. Raudino, D. Berti, R. Giorgi, P. Baglioni</i>
17.45-19.30		<i>Presentazione Progetti di Ricerca Tavola Rotonda sulla Ricerca e sulla Valutazione della Ricerca</i>
19.30		<i>Pizza Party</i>
21.00-23.00		<i>Concerto a cura del Coro e Orchestra dell'Università del Piemonte Orientale</i>

<u>25 Giugno 2013</u>		
Sessione 3: Modeling e Chimica Computazionale		
<i>Chair:</i>		
9.00-9.45	PL2	IN SILICO DESIGN OF DYE SENSITIZED SOLAR CELLS
		<i>Carlo Adamo (Ecole Nationale Supérieure de Chimie, Paris)</i>
9.45-10.00	3O1	THE STRUCTURE OF IONIC LIQUIDS FROM A MOLECULAR PERSPECTIVE: RECENT THEORETICAL AND EXPERIMENTAL RESULTS
		<i>E. Bodo, R. Caminiti</i>
10.00-10.15	3O2	INFRARED AND RAMAN SPECTRA OF CRYSTALLINE SYSTEMS THROUGH AB INITIO SIMULATIONS
		<i>L. Maschio, B. Kirtman, M. Rerat, R. Orlando, R. Dovesi</i>
10.15-10.30	3O3	STOCHASTIC SIMULATIONS OF MINIMAL CELL MODEL SYSTEMS
		<i>F. Mavelli</i>
10.30-10.45	3O4	THE UNUSUAL CURRENT DENSITY PATTERNS OF ALTAN-MOLECULES
		<i>G. Monaco, R. Zanasi</i>
10.45-11.00	3O5	MODELING SUPRAMOLECULAR ORGANIZATION AND CHARGE TRANSPORT IN DISCOTIC LIQUID CRYSTALS
		<i>S. Orlandi, M. Lamarra, L. Muccioli, C. Zannoni</i>
11.00-11.20		<i>Coffee-break</i>
<i>Chair:</i>		
11.20-11.45	KN3	NEW VIRTUAL INSTRUMENTS FOR MOLECULAR SCIENCE: THE MULTIFREQUENCY SPECTROMETER
		<i>V. Barone, M. Biczysko, J. Bloino, C. Cappelli</i>
11.45-12.00	3O6	MOLECULAR SIMULATIONS OF GAS ADSORPTION IN DIAMOND-LIKE POROUS AROMATIC FRAMEWORKS (PAF): CH₄, H₂ AND CO₂
		<i>A. Fraccarollo, L. Canti, M. Cossi</i>
12.00-12.15	3O7	THEORETICAL AND COMPUTATIONAL TOOLS TO UNDERSTAND THE SPECTROSCOPY AND REACTIVITY OF BIO-MOLECULES
		<i>A. Petrone, P. Cimino, N. Rega</i>
12.15-12.30	3O8	INVESTIGATING WEAKER HYDROGEN BONDS: THE CASE OF FROZEN, QUANTUM AND T>0 K AMMONIA CLUSTERS
		<i>P.E. Janiero-Barral, M. Patrone, M. Mella, E. Curotto</i>

12.30-12.45	309	MODELLING JUNCTION DOMAINS IN POLY(VINYL ALCOHOL) CHEMICALLY CROSS-LINKED HYDROGELS BY MOLECULAR DYNAMICS
		<i>E. Chiessi, A. Lonardi, G. Paradossi</i>
12.45-13.00	3010	NEW FORCE FIELD FOR FAST MOLECULAR DYNAMICS SIMULATIONS IN FLEXIBLE ALUMINOSILICATES
		<i>A. Gabrieli, M. Sant, P. Demontis, G.B. Suffritti</i>
13.00-14.30		<i>Pranzo a Buffet</i>

Sessione 4: Materiali per l'Energia e per la Catalisi (I)

<i>Chair:</i>		
14.30-14.55	KN4	IMPROVING DSSC PERFORMANCES THROUGH COMBINED EXPERIMENTAL AND COMPUTATIONAL APPROACHES
		<i>C. Bisio, G. Gatti, M. Cossi, L. Marchese</i>
14.55-15.10	4O1	DYNAMICS OF P3HT AND PHASE SEPARATION IN MATERIALS USED IN ORGANIC SOLAR CELLS
		<i>M. Geppi, F. Martini, S. Borsacchi, S. Spera</i>
15.10-15.25	4O2	THE USE OF LIGHT FOR THE PREPARATION OF POLYMER ELECTROLYTES FOR DYE-SENSITIZED SOLAR CELLS
		<i>F. Bella, C. Gerbaldi, S. Bianco, E. Tresso, R. Bongiovanni</i>
15.25-15.40	4O3	STATE OF THE ART AND PERSPECTIVES OF INORGANIC PHOTOVOLTAIC: THE RESEARCH ACTIVITY AT MIBSOLAR CENTER
		<i>S. Binetti, A. Le Donne, S. Marchionna, S. Tombolato, P. Garattini, M. Acciarri</i>
15.40-15.55	4O4	A NOVEL BIO-INSPIRED APPROACH TO IMPROVE SOLAR CELLS PHOTON TO CURRENT CONVERSION EFFICIENCY
		<i>E. Gatto, A. Quatela, M. Caruso, R. Tagliaferro, M. de Zotti, F. Formaggio, C. Toniolo, A. di Carlo, M. Venanzi</i>
15.55-16.10	4O5	MICROSCOPIC ORIGIN OF EFFICIENT CHARGE SEPARATION IN ORGANIC P3HT:PCBM SOLAR CELLS
		<i>G. D'Avino, S. Mothy, L. Muccioli, C. Zannoni, L. Wang, J. Cornil, D. Beljonne, F. Castet</i>
16.10-16.30		<i>Coffee-break</i>
<i>Chair:</i>		

16.30-16.55	KN5	COLLOIDAL INORGANIC NANOCRYSTALS AS BUILDING BLOCKS TO ENGINEER NEW FUNCTIONS IN MATERIALS FOR ENERGY CONVERSION
		<i>E. Fanizza, M. Corricelli, E. Di Mauro, A. Panniello, C. Ingrosso, R. Comparelli, M. Striccoli, M. L. Curri, A. Agostiano</i>
16.55-17.10	4O6	UNVEILING EXTENDED DISORDER IN $Ce_{1-x}Gd_xO_{2-x/2}$ SOLID ELECTROLYTE FOR SOFC USING PDF AND ANOMALOUS PDF
		<i>M. Scavini, M. Coduri, M. Brunelli, M. Allieta, P. Masala, C. Ferrero</i>
17.10-17.25	4O7	LOW-TEMPERATURE PROTONIC CONDUCTIVITY MECHANISM IN FULLY DENSE NANOMETRIC TiO_2
		<i>I.G. Tredici, F. Maglia, P. Mustarelli, C. Ferrara, A. Resmini, G. Spinolo, U. Anselmi-Tamburini</i>
17.25-17.40	4O8	DYE-LOADING INFLUENCE ON PERFORMANCES OF FLUORENONE/ZEOLITE L LIGHT HARVESTER
		<i>L. Gigli, R. Arletti, E. Fois, G. Tabacchi, S. Quartieri, G. Vezzalini, J.G. Vitillo</i>
17.40-17.55	4O9	NEW LIQUID CRYSTALLINE THIENOVIOLOGENS AS ADVANCED MULTIFUNCTIONAL MATERIALS
		<i>A. Beneduci, S. Cospito, B. de Simone, D. Imbardelli, M. la Deda, G. Chidichimo</i>
18.00-19.30		<i>Tavola Rotonda sulla Didattica</i>
21.30-23.00		<i>Visita Guidata alla Cittadella di Alessandria</i>

26 Giugno 2013

Sessione 5: Materiali per l'Energia e per la Catalisi (II)

Chair:

9.00-9.45	PL3	CATALYST DESIGN STRATEGIES FOR ENERGY EFFICIENCY AND SUSTAINABILITY
		<i>R. Raja (University of Southampton, UK)</i>
9.45-10.00	5O1	COPPER CATALYTICALLY ACTIVE SITES IN SILICA-CONTAINING MATRICES. AN EPR STUDY
		<i>A. Barbon, F. Zaccheria, N. Ravasio</i>
10.00-10.15	5O2	SELF-ASSEMBLY OF A SUPRAMOLECULAR BI-LAYER FOR PHOTO-INDUCED WATER SPLITTING
		<i>G. Zappalà, F. Puntoriero, A. Sartorel, M. Bonchio, S. Campagna, A. Licciardello</i>
10.15-10.30	5O3	MICROPOROUS MATERIALS FOR GAS AND MONOMER CAPTURE

		<i>A. Comotti, S. Bracco, I. Bassanetti</i>
10.30-10.45	504	THERMODYNAMIC AND KINETIC PROPERTIES OF THE LiBH₄-MgH₂ AND LiBH₄-MgH₂-LiAlH₄ SYSTEMS FOR SOLID-STATE HYDROGEN STORAGE
		<i>C. Milanese, A. Girella, V. Berbenni, G. Bruni, S. Soru, S. Garroni, S. Enzo, G. Mulas, J. Jepsen, C. Pistidda, J. Bellosta von Colbe, M. Dornheim, T. Klassen, A. Marini</i>
10.45-11.00	505	CdS AND M_xZn_{1-x}S CATALYSTS FOR HYDROGEN PRODUCTION: SYNTHESIS AND CHARACTERIZATION
		<i>E. Balantseva, G. Berlier, P. Davit, A.M. Ferrari, G. Trunfio, L. Spadaro, F. Arena, S. Coluccia</i>
11.00-11.20		<i>Coffee-break</i>
<i>Chair:</i>		
11.20-11.45	KN6	IR SPECTROSCOPY AND MODELLING OF ADSORBED MOLECULES: ADVANCES IN PROBING MORPHOLOGY, TOPOGRAPHY AND REACTIVITY OF TiO₂ NANOPARTICLES
		<i>C. Deiana, G. Tabacchi, Y. Sakhno, V. Maurino, E. Fois, G. Martra</i>
11.45-12.00	506	TiO₂ NANOPARTICLES PRODUCED BY LASIS AND HYDROTHERMAL SYNTHESIS: EFFECTS OF PARAMETERS ON CRYSTAL PHASE AND MORPHOLOGY
		<i>M. Ferretti, E. Sanguineti, M.M. Carnasciali, T. Montanari, A. Casu, V. Caratto</i>
12.00-12.15	507	DOPED TITANIA NANOCRYSTALS EXPLAINED BY EXPERIMENTAL AND DFT CHARACTERIZATIONS
		<i>M. Ceotto, L. Lo Presti, G. Cappelletti, L. Falciola, D. Meroni, F. Spadavecchia, S. Ardizzone</i>
12.15-12.30	508	HALLOYSITE BASED MATERIAL FOR ENHANCED SOLUBILIZATION
		<i>G. Cavallaro, G. Lazzara, S. Milioto</i>
12.30-12.45	509	PHOTOINDUCED PHENOMENA IN SINGLE WALLED CARBON NANOTUBE/CONJUGATED POLYMER LANGMUIR-SCHAEFER FILMS
		<i>G. Giancane, V. Sgobba, A. Operamolla, O.H. Omar, F. Babudri, G.M. Farinola, D.M. Guldi, L. Valli</i>
12.45-13.00	5010	SERS INVESTIGATION OF INTERFACES IN CORE-SHELL QUANTUM DOTS WITH VARIABLE SHELL COMPOSITION
		<i>F. Todescato, A. Minotto, F. Signorini, J.J. Jasieniak, R. Bozio</i>
13.00-14.30		<i>Pranzo a Buffet</i>

14.30-16.00			Sessione Poster		
16.00-17.00		<i>Assemblea dei Soci</i>			
17.00-24.00		<i>Tour e Cena Sociale</i>			
<u>27 Giugno 2013</u>					
Sessione 6: Processi Biologici					
<i>Chair:</i>					
9.00-9.45	PL4	SALT, WATER AND PHYSICAL CHEMISTRY			
		<i>B. Ninham (Australian National University)</i>			
9.45-10.00	601	LOCALIZED SURFACE PLASMON RESONANCE STUDY OF PROTEIN ADSORPTION: LONG AND SHORT RANGE FORCE EFFECT AT SOLID-LIQUID INTERFACES			
		<i>N. Gianblanco, E.M. Langhammer, G. Marletta</i>			
10.00-10.15	602	SPECTROSCOPIC CHARACTERIZATION OF 2,6-DIMETHOXYPHENOL MEDIATOR RADICALS FORMED IN THE LACCASE BIOCATALYTIC MECHANISM			
		<i>M.C. Baratto, A. Martorana, R. Vazquez-Duhalt, R. Basosi</i>			
10.15-10.30	603	HYDRATION DYNAMICS IN BIORELEVANT SYSTEMS: INSIGHTS FROM EXTENDED DEPOLARIZED LIGHT SCATTERING (EDLS) EXPERIMENTS			
		<i>M. Paolantoni, P. Sassi, L. Comez, L. Lupi, D. Fioretto, A. Morresi</i>			
10.30-10.45	604	LIGAND INTERACTIONS IN THE DISTAL HEME POCKET OF TRUNCATED HEMOGLOBINS: ROLES OF THE DISTAL RESIDUES			
		<i>E. Droghetti, F. Nicoletti, A. Feis, B.D. Howes, J.P. Bustamante, D. Estrin, C. Verde, A. Boffi, G. Smulevich</i>			
10.45-11.00	605	MOLECULAR MECHANISMS IN DRUG RESEARCH: INSIGHT BY PHYSICO-CHEMICAL TOOLS			
		<i>G. Ponterini</i>			
11.00-10.20		<i>Coffee-break</i>			
<i>Chair:</i>					
11.20-11.45	606	HUMAN MYOGLOBIN ISOFORMS: SINGLE MUTATION FAR FROM THE ACTIVE SITE AFFECTS DYNAMICS AND NO REACTIVITY			
		<i>M.A. Scorciapino, E. Spiga, A. Vezzoli, S. Mrakic-Sposta, R. Russo, B. Fink, M. Casu, M. Gussoni, M. Ceccarelli</i>			

11.45-12.00	607	STUDY OF COPPER TRANSPORT MECHANISM IN HUMAN COPPER ATPASES (ATP7A/B)
		<i>F. Tadini-Buoninsegni, G. Bartolommei, M.R. Moncelli</i>
12.00-12.15	608	HOFMEISTER CHALLENGES: ION BINDING AND CHARGE OF THE BSA PROTEIN AS EXPLICIT EXAMPLES
		<i>L. Medda, B. Barse, F. Cugia, D.F. Parsons, B.W. Ninham, M. Monduzzi, A. Salis</i>
12.15-12.30	609	X-RAY INDUCED PHOTODAMAGE IN PROTEINS: A RAMAN-ASSISTED BIOCRYSTALLOGRAPHIC STUDY
		<i>A. Merlino, M. Fuchs, F. Dworkowski, M. Caterino, A. Vergara</i>
12.30-12.45	6010	ANALYTICAL MODEL AND MULTISCALE SIMULATIONS OF AB PEPTIDE AGGREGATION IN LIPID MEMBRANES
		<i>M. Pannuzzo, D. Milardi, A. Raudino, M. Karttunen, C. La Rosa</i>
12.45-13.15		<i>Cerimonia di Chiusura</i>