

Consorzio Interuniversitario per lo Sviluppo dei Sistemi a Grande Interfase

Report 2017

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IV

CSGI Research Activity

Outline

CSGI (Research Center for Colloids and Nanoscience) was established in Firenze, in December 1993. It has been officially recognized by the Italian Government in 1994, and is under the supervision and control of the Italian Ministry for University and Scientific Research (MIUR). Since 1995, CSGI began its scientific activity, devoted to basic research and to the development of high-tech new processes. It is also supporting the activities of the small and medium size business industrial companies, that cannot afford the financial costs of an independent research activity.

In the last years, CSGI has sponsored several different research programs, mainly supported by European Union grants (such as Nanorestart, Dna-Trap, Issflow, ShaleXEnvironment, Bioclean, Icarus), and partly also by other international and national Institutions, such as the Italian PRIN, PNR, FISR, FIRB, POR FESR and so forth.

CSGI has signed numerous contracts that involve about 75 national and international industrial companies, and some highly qualified research Centers, such as: Procter & Gamble, Siemens, Tecnotessile SpA, Massachusetts Institute of Technology, Bayer-Schering, L'Oreal, Solay, Eni SpA, bioMérieux Italia SpA, Lamberti SpA, Giuliani SpA, CTG Italcementi, King Saud University, Martelli Srl, Rifinizione S. Stefano, AMSA, Pierre Fabre, Farmabios, Fater SpA, University of Florida, È Così, Lachesis, MBN SpA, Novartis, W.A.D.A., Morphotec, Perkin Elmer, Grünenthal Gmbh, Comune di Firenze, Teletron Euroricerche, VTT, etc... The main results of these collaborations have brought to several International Patents and research agreements.

CSGI has reached a very qualified standard, and its level has been acknowledged abroad, in several fields. For example, CSGI is a leader in many applications of Nanotechnology, in the conservation of cultural heritage, and in the making of nanophasic powders (with MBN) to produce special materials for aeronautics, high resistance coatings, etc. CSGI supports the local authorities for the safeguard and conservation of works or art ("Sovrintendenze Artistiche") in Tuscany and other Italian districts, with technologies that have been developed for this aim. Similar actions promoted by the Mexican Federal Government for the conservation of Calakmul, Campeche), have been conducted in association with Mexican museums and conservation institutions.

CSGI is also very active in the training of specialized researchers, has granted several fellowships, PhD supporting programs, post-doc grants, and other education projects, and has organized several national and international meetings and symposia. During the years 2014-2016, CSGI has issued 14 PhD scholarships, 39 fellowships, and 62 post-doc grants, and is actively participating in one European Master Program: IMES (International Master on Bioenergy and Environment). CSGI has co-sponsored national and international congresses (International Workshop on Dynamic Crossover Phenomena in Water and Other Glass-forming Liquids and CSGI National Meeting).

The CSGI financial plan is solid, with a strong growth of its financial assets, mainly due to EU funding.

The main topics of CSGI research activity are:

• development of processes to produce: nanophasic systems (i) innovative textiles, (ii) nanophasic alloys, (iii) ceramics and nanophasic or nanostructured composites (with low temperature and low energy costs);

• setup of new additives for cement products and cement formulations. These projects are mainly carried out in collaboration with CTG-Italcementi and MIT, and are aimed at investigating and optimizing (i) the cement hydration process and the production of new additives, (ii) ceramics-like materials for the cement-related industry;

• formulation of dispersions in fluids, emulsions and inverted emulsions (paints, adhesives, sealing materials, detergents, etc.);

• development of systems for the confinement of proteins and for the controlled release of pharmaceutics;

• development of food-related industrial processes (for example the treatment of milk and milk derivatives in supercritical phase);

• development of innovative procedures for the conservation and restoration of works of art (paintings, frescoes and stone-based materials).

CSGI is a world leader in this research activity, and is involved in a significant campaign for the recovery of archaeological treasures in Mexico (Calakmul), the largest Maya sites, and in several other countries (Cile, Argentina, Sweden, Spain, India, Egypt, Israel, Romania, etc.).

Fields of Interest

- Nanostructured and ultrafine materials.
- Structure and dynamics of supramolecular assemblies (monolayers, micelles, liposomes, microemulsions, Langmuir-Blodgett films, host-guest systems).
- Nanophasic ternary oxides.
- Structural analysis of biomolecules in solution, interaction processes, recognition of ligands with macromolecular surfaces, theoretical and experimental analysis of cellular metabolism, interactions between metals and ligands, characterization of the interaction sites.
- Formulation of nanophasic systems.
- Innovative processes for the conservation and restoration of cultural heritage (stone materials, wood materials, paintings, frescoes, paper, photographic material).

National Agency for the evaluation of Quality of Research (2011-2014): CSGI ranking

CSGI was one of the 9 Consortia that voluntary submitted their candidature, for the second time in a raw, to the Italian evaluation of universities and research centers: Valutazione della Qualità della Ricerca (VQR), an exercise to evaluate the quality of the research efforts in the period 2011-2014. The report was produced by Agenzia Nazionale di Valutazione del sistema Universitario e della Ricerca (ANVUR), an Italian national agency for the Italian research qualification. VQR 2006-2010 and 2011-2014 resulted in the largest-scale evaluations of research in Italy's history.

The VQR examined research outcomes in 14 disciplinary areas of study published between 2011 and 2014 by 96 universities, 18 research centers and 19 other institutions to identify the significance of the Italian research output and how it compares globally. By reviewing a significant number of Italian research outcomes,

ANVUR could gain a greater understanding of Italian research strengths, impact and neglected fields of study.

CSGI ranked in the first position among the other Italian Consortia for Chemical Sciences (Area 03) for the period 2011-2014.

In the disciplines related to Chemical Sciences (the core of the CSGI research), CSGI resulted as excellent (about 85% of the submitted products were judged as excellent and the remaining products were classified as good). The final indicators for the research and the third mission are well above the average values for Consortia in the same categories.

Structure and Organization of CSGI

Management Offices President, Council, Director, Audit Council, Technical-Scientific Board.

Director of CSGI Prof. Piero Baglioni, Department of Chemistry, University of Florence.

President of CSGI Prof. Giovanni Marletta, Department of Chemical Sciences, University of Catania.

Website http://www.csgi.unifi.it/

Foundation December 21st, 1993

Official recognition by the Italian Government November 15th, 1994 (G.U. Nr. 267)

Academic Units and Associated Centers

- University of Florence (headquarter)
- Scuola Normale Superiore in Pisa
- University of Bari "Aldo Moro"
- University of Bergamo
- University of Catania
- University of Cagliari
- University of Molise (Campobasso)
- University of Naples "Federico II"
- University of Pavia
- University of Siena



- Laboratory CSGI of Treviso
- Opificio delle Pietre Dure
- Polytechnic Institute of Milan
- University of Bologna
- University of Brescia
- o University of Milan, Bicocca
- o University of Palermo
- o University of Perugia
- o University of Rome, La Sapienza
- o University of Rome, Tor Vergata
- o University of Rome TRE
- University of Venice

Personnel

CSGI gathers about 300 researchers including Full Professors, Associate Professors, University Researchers, that belong to the academic members.

Moreover, CSGI employs 75 researchers and 4 administration employees on its own. Several PhD and post-doc students are financially supported through CSGI fellowships. CSGI hosts researchers hired by industrial companies for training and specific research activities, in the framework of various European projects.

CSGI owns two research Laboratories, located in Vascon di Carbonera (Nanophases Laboratory).

Previous and Current Academic Collaborations

ANU - Australian National University Argonne National Laboratory Aston University (Birmingham) Brookhaven National Laboratory California Institute of Technology - CalTech Centro di Istochimica del CNR di Pavia Chalmers University of Technology CNIC - Centro Nacional de Ivestigaciones Cientificas (Cuba) CNR - Consiglio Nazionale delle Ricerche CNRS - Centre National de la Recherche Scientifique Collège de France Columbia University CPMCRI - California Pacific Medical Center Research Institute-, San Francisco CSIC (Sevilla) East China Normal University (Shangai) École Normale Supérieure (Lion) Escuela Superior Politecnica del Chimborazo ETH Zürich - Eidgenössische Technische Hochschule Zürich Hahn-Meitner Institut (Berlin) Hull University Inst. Nat. Polytechnique de Lorraine (Nancy) Inst. Science des Matériaux Inst. Scientific Instruments (Czech Rep.) Institut Laser Technology ITER - International Thermonuclear Experimental Reactor Laboratoire Leon Brillouin (Saclay) Lehstul Fertigungstechnologie Massachusetts Institute of Technology Max Planck Institut (Berlin) Max Plank Institut Biofisica (Francoforte) Museum of Fine Arts (Boston) Nuclear Research Institute (Prague) Oak Ridge National Laboratory Oklahoma State University Risø National Laboratory Technical University di Budapest Technische Universität Darmstadt Tekniska Hogskolan I Luleå

The Getty Conservation Institute Tufts University UCLA - University of California Los Angeles Università degli Studi della Calabria Università degli Studi di Bari Università degli Studi di Camerino Università degli Studi di Chieti Università degli Studi di Ferrara Università degli Studi di Genova Università degli Studi di Milano Università degli Studi di Padova Università degli Studi di Palermo Università degli Studi di Parma Università degli Studi di Pisa Università degli Studi di Salerno Università degli Studi di Siena Università degli Studi di Torino Università degli Studi di Trento Università degli Studi di Urbino Universitad de Santiago de Compostela Universitad del Salvador Universitad Estadual de Campinas Universität Gesamthoschule Kassel Universität Heidelberg Universität Konstanz Université "Louis Pasteur" (Strasbourg) Université de Bourgogne Université de Grenoble Université de Montpellier II University College (London) University of Berkeley University of Bristol University of Cambridge University of Detroit University of East Anglia University of Houston University of Leiden University of Lund University of South Florida University of Sydney University of Valladolid University of York Weizmann Institute (Israel)

Previous and Current Industrial Partners

3M Alcea Alfa Test Alfa Wasserman Angelini Ansaldo Aprilia Ascor chimici Ausimont Bigagli Biokimica SpA bioMérieux Italia SpA Bioscreen Technology srl Bitossi BTG-Holland Chemia Chiesi Farmaceutici SpA Chimet S.p.A. Comune di Firenze Consorzio delle Buone Idee Cover D'Appolonia Dynamotive Elf-Atochem ENEA (Energy Department - Casaccia) Eniricerche Eni SpA Enitecnologie EUBIA (Bruxelles) Fater SpA Flory's Getty Conservation Institute Glaxo-Wellcome Icmese INASCO-Hellas (Int. Aerosp. Sci. Corp.) Industrial Materials Technology GmbH Industrie Casearie Podda Ineti Institute for the Care of Hystorical Monuments (Prague) Instituto Nacional de Antropología e Historia -INAH International Broker Inver

IRBM Italcementi SpA Italfarmaco JRC (Joint Research Centre of the European Commission) Kucept Ltd (UK) Lamberti SpA Ely-Lilly Lima Lombardia Mapei Mariplast Martelli Srl MBN Nanomaterialia Merk Microtec (Germany) Nanovector Srl Nicox Novuspharma Omrod Diesel (UK) Orion Pharma Pharmacia-Upjon (USA and Sweden) Pharmaness Philips Procarta Biosystems Ltd Procter & Gamble Rifiniture BP S.I.F.I. Sem Siemens AG Sigma-tau Sintech SIR Industriale Sirio Panel Solvay Soprintendenze ai Beni Artistici e Storici di: FI-PO-PT, SI-GR, PI-LU-MS Tecnotessile SpA Tecrea Ltd (UK) TIL (Tooling International Ltd UK) TNO (Netherlands) Transfergomma (Padova) VTT (Finland). WIP (Germany)

CSGI Patents

- Baglioni Piero, Dei Luigi, Ferroni Enzo, Giorgi Rodorico "Sospensioni stabili di idrossido di calcio". Italian Patent FI/96/A000255, deposit date 31/10/1996.
- Matteazzi Paolo, Baglioni Piero, Basset Diego "Process for Recycling, by Milling, Solid Industrial Waste and Materials at the end of their Service Life". European Patent Application 97203735.2, Priority IT96 FI96A000280.
- Grassi Giuliano, Chiaramonti David, Baglioni Piero "Apparato a combustione di etanolo o miscele etanolo per cucine, stufe e illuminazione a uso domestico". Italian Patent FI/98/A42, deposit date 24/02/1998.
- 4) Ambrosone Luigi, Ceglie Andrea "Software per l'analisi grafica e numerica di dati di Risonanza Magnetica Nucleare per la determinazione della polidispersità di emulsioni". Italian Patent FI99A000044, deposit date 09/03/1999.
- 5) Baglioni Piero, Carretti Emiliano, Dei Luigi "Microemulsioni ed emulsioni di olio in acqua, loro uso per la solubilizzazione di resine polimeriche e impacchi contenenti detti microemulsioni o emulsioni". Italian Patent FI99A000071, deposit date 02/04/1999.
- 6) Baglioni Piero, Fratini Emiliano, Ricceri Riccardo, Sarti Giuseppe, Chiaramonti David "Engine fuels consisting of an emulsion comprising mineral and/or natural oils, their preparation and use in internal combustion engine". PCT International Application WO n. 99936473.0 del 02/07/1999.
- Baglioni Piero, Bardi Ugo, Bonini Massimo New method for the production of solid powder and films by compartimentalised solution thermal spraying (CSTS). European Patent Application EP 00-105673.8, deposit date 17/03/2000.
- Angelico Ruggero, Ceglie Andrea, Hochoeppler Alejandro, Palazzo Gerardo, Stefan Alessandra – "Macroemulsioni acqua-in olio a lunga stabilità, loro preparazione ed uso". Patent Query N. FI2001A000016, Italian Patent N. 0001328470, deposit date 29/01/2001.
- 9) Baglioni Piero, Dei Luigi, Fratoni Laura, Lo Nostro Pierandrea, Moroni Michelangelo "Processo per la preparazione di nano e microparticelle di ossidi e idrossidi di metalli del secondo gruppo e di transizione, nano e microparticelle così ottenute e loro impiego in campo ceramico, tessile e cartario". Patent Query N. FI2002A000052, deposit date 28/03/2002 EP 03745367.7.
- Baglioni Piero, Dei Luigi, Giorgi Rodorigo, Claudio Vinicius Schettino "Basic Suspensions their Preparation and Use in Processes for Paper Deacidification". European Patent Application EP 02714088.8, deposit date 15/01/2002.
- 11) Ambrosone Luigi, Ceglie Andrea "Materiale assorbente e suoi usi nei processi di bonifica di falde acquifere inquinate da prodotti chimici". Patent Query FI2003A000236, deposit date 11/09/2003.
- Ambrosone Luigi, Ceglie Andrea "Gel stabili contenenti gelatina". Patent Query N. FI2003A000237, deposit date 11/09/2003.

- 13) Baglioni Piero, Dei Luigi, Fratoni Laura, Lo Nostro Pierandrea, Moroni Michelangelo "Preparation of nano and micro-particles of group II and transition metals oxides and hydroxides and their use in the ceramic, textile and paper industries". PCT Int. Appl. (2003), 10 pp. CODEN: PIXXD2 WO 2003082742 A2 20031009 CAN 139:278604 AN 2003:796605.
- Fratoni Laura, Lo Nostro Pierandrea "Composizione detergente a base di un estere dell'acido L-ascorbico". Patent Query N. TO2003A001032, deposit date 22/12/2003.
- 15) Baglioni Piero, Dei Luigi, Giorgi Rodorico, Ninham Barry W. "Process for preparing nano- and micro-sized particles of inorganic compounds". European Patent Application EP 04101822.7, deposit date 29/04/2004.
- 16) Ambrosi Moira, Baglioni Piero, Bonini Massimo, Fratini Emiliano "Nanoparticelle monodisperse di ossidi ed idrossidi metallici e loro applicazione nei settori tessile, cartario e ceramico". Patent Query FI 2006A000313 – RIF. 7845 PTIT, deposit date 11/12/2006.
- 17) Baglioni Piero, Ambrosi Moira, Dei Luigi, Faneschi Mauro, Mancioli Luciano, Santoni Sergio – "Ceramic products comprising nanoparticles of zirconium hydroxide and/or glass frits". Patent Query 7303 PTEP/2006 EP06112439.2, deposit date 10/04/2006.
- 18) Ceglie Andrea, Venditti Francesco, Lopez Francesco, Palazzo Gerardo, Colafemmina Giuseppe, Angelico Ruggero, Ambrosone Luigi – "Materiale adsorbente contenente tensioattivo cationico, sua preparazione ed uso per la rimozione di metalli da soluzioni acquose". Patent Query N. FI 2006 A000113 – RIF. 7490 PTIT, Italian Patent N. 0001368154/2009, deposit date 10/05/2006.
- 19) Ballistreri Alberto, Cambria Maria Grazia, Carnemolla Giovanni Marco, Guglielmino Salvatore Pietro Paolo, Impallomeni Giuseppe, Nicolo Marco Sebastiano – "Production of biodegradable plastics from Brassica carinata oil with high content of erucic acid and from very long chain fatty acids". Italian Patent IT 1392236, deposit date 13/10/2008.
- 20) Ballistreri Alberto, Cambria Maria Grazia, Carnemolla Giovanni Marco, Guglielmino Salvatore Pietro Paolo, Impallomeni Giuseppe, Nicolo Marco Sebastiano – "Production of biodegradable plastics from Brassica carinata oil with high content of erucic acid and from very long chain fatty acids". World Organization Patent WO 2010044118 Priority IT 2008-RM545.
- 21) Hochkoeppler Alejandro, Baglioni Piero, Stefan Alessandra "Espressione batterica di un gene artificiale per la produzione di CRM 197 e derivati". Patent Query FI 2009A000137 – RIF. 9741 PTIT, deposit date 25/06/2009.
- 22) Primiceri Giuseppe, Roda Elena, Stefan Alessandra, Panizza Lucio, Hochkoeppler Alejandro – "Enzyme composition for reducing the release of pharmaceutical active ingredients into the environment". WO/2009/138455A1.

- 23) Hochkoeppler Alejandro, Roda Elena, Panizza Lucio, Stefan Alessandra "Method for preventing and controlling biofouling on marine objects". WO/2010/145905A.
- 24) Panizza Lucio, Roda Elena, Stefan Alessandra, Hochkoeppler Alejandro "Method for preventing and controlling organisms that infest aqueous systems." WO/2010/145988A1.
- 25) Smets Johan, Pintens An, Keijzer Olav Pieter Dora Tony, Bodet Jean-Francois, Lebron Ariel, Fratini Emiliano, Vannucci Chiara, Ambrosi Moira, Baglioni Piero, Guinebretiere Sandra Jaqueline, Yan Nianxi, Liu Hongwei – "Encapsulates". Attorney's Docket No. 11547P – 21/04/2010.
- 26) Fernandez Prieto Susana, Smets Johan, Aouad Yousef Georges, Wevers Jean, Baglioni Piero, Ambrosi Moira, Vannucci Chiara – "Particles". Attorney's Docket No. 11812P2, 15/04/2011.
- 27) Angelico Ruggero, Lampis Sandrina, Monduzzi Maura, Ceglie Andrea "Metodo innovativo per la "plastificazione" di grassi vegetali". Italian Patent FI2012A000186, deposit date 19/09/2012.
- 28) Paduano Luigi, D'Errico Gerardino, Montesarchio Daniela, Vitiello Giuseppe, Mangiapia Gaetano, Luchini Alessandra, Irace Carlo, Colonna Alfredo, Santamaria Rita – "Nanoparticelle ibride magnetite-oro funzionalizzate con struttura nucleo-guscio". Italian patent, deposit date 19/10/2012.
- 29) Ranieri Rossi, Daniela Giustarini "Metodo per la misura del glutatione su sangue prelevato tramite digitopuntura" Italian Patent N. 0001420029 deposit date 18/06/2013.
- 30) Piero Baglioni, Stefano Del Buffa, Francesca Ridi, Massimo Bonini "Materiale per la rigenerazione dei tessuti ossei contenente minerali argillosi aventi morfologia nanotubolare e stronzio". Italian Patent FI2013A000240, deposit date 15/10/2013.
- Bettini Ruggero, Hochkoeppler Alejandro, Melegari Cecilia, Primiceri Giuseppe, Stefan Alessandra – "Composizioni farmaceutiche con ridotto impatto ambientale." Italian patent IT 0001415653, deposit date 12/05/2015.

CSGI Registered Trade Marks

- 1) Nanorestore® International Class 01,37,40 FI2008C00067527508 RIF. 19558
- Nanorestore Paper[®] International Class 01, 16, 40 FI2011C0009935263 RIF. 27175
- Nanorestore Gel® International Class 01, 03, 37 Registration n. 12696308 del 12/08/2014 RIF. 30346

- Nanorestore Cleaning[®] International Class 01, 03, 37 Registration n. 013603006 del 07/05/2015 RIF. 30836
- Nanorestore Plus[®] International Class 01, 37, 40 Registration n. 014414262 del 30/11/2015 RIF. 30836

Prospective CSGI Activity in 2017-2018

CSGI is involved in several European projects (FP7 and H2020), in several international and national projects, and in collaborations with industries and SME (small and medium enterprises).

CSGI is developing its own research activity to optimize the application of research projects inspired by the urging demands of small and medium size companies.

CSGI is actively working to offer a valid support to the Italian industrial system to set and develop of projects and pre-industrial processes.

List of Publications 2014-2016

- 1,2-Benzisothiazole Derivatives Bearing 4-, 5-, or 6-Alkyl/arylcarboxamide Moieties Inhibit Carbonic Anhydrase Isoform IX (CAIX) and Cell Proliferation under Hypoxic Conditions. Coviello, V; Marchi, B; Sartini, S; Quattrini, L; Marini, AM; Simorini, F; Taliani, S; Salerno, S; Orlandi, P; Fioravanti, A; Di Desidero, T; Vullo, D; Da Settimo, F; Supuran, CT; Bocci, G; La Motta, C. *Journal Of Medicinal Chemistry* 59, 6547-6552 (2016).
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- Altamura, E.; Milano, F.; Trotta, M.; Omar, O.H.; Stano, P.; Mavelli, F. XXIII Congresso Nazionale SIPBA, in Cortona (Italy), 18-21/09/2016. Oral presentation.
- Altamura, E.; Milano, F.; Trotta, M.; Omar, O.H.; Stano, P.; Mavelli, F. Syschem 2016, Valtice Chateau (CZ), 08-12/05/2016. Oral presentation.
- 3. Ancona, A.; Sportelli, M.C.; Picca, R.A.; Izzi, M.; Di Maria, A.; Volpe, A.; Lugarà, P.M.; Cioffi, N. EMRS2016 Spring Meeting, Lille (France), 01-06/05/2016, Symposium C. Oral communication.
- Angelico, R.; Ceglie, A.; Sacco, P.; Ripoli, M. 30th Conference of the European Colloid and Interface Society (ECIS 2016), Roma (Italy), 04-09/09/2016. Poster.
- Angelico, R.; Ceglie, A.; Sacco, P.; Ripoli, M. 30th Conference of the European Colloid and Interface Society (ECIS 2016), Roma (Italy), 04-09/09/2016. Poster.
- Angelico, R.; Gentile, L.; Ranieri, G.A.; Oliviero Rossi, C. Organizing Molecular Matter A Soft Matter Symposium, Lund (Sweden), 19-26/06/2016. Oral presentation.
- Angelico, R.; Gentile, L.; Ranieri, G.A.; Oliviero Rossi, C. XLIV Congresso Nazionale della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Oral presentation.
- Angelico, R.; Oliviero Rossi, C.; Caputo, P.; Calandra, P.; Mezzi, A.; Teltayev, B. 30th Conference of the European Colloid and Interface Society (ECIS 2016), Roma (Italy), 04-09/09/2016. Poster.
- Baglioni, P. 12th International Conference on Colloid and Surface Chemistry, Iasi (Romania), 16-18/05/2016. Invited lecture.
- Baglioni, P. Annual Surface and Materials Chemistry Symposium 2016, Gothenburg (Svezia), 8-10/11/2016. Invited lecture.
- 11. Baglioni, P. Chemistry of Art Reconstruction, Accademia Reale Olandese, Van Arkel Award, Amsterdam (Olanda), 26/05/2016. Plenary lecture.
- Baglioni, P. ECIS 2016, 30th International conference of the European Colloid and Interface Society, Rome, 04-09/09/2016. Overbeek award plenary lecture.
- 13. Baglioni, P. Formula VIII, Barcelona (Spagna), 04-07/07/2016. Plenary lecture.
- Baglioni, P. Italy-Mexico, bilateral meeting on study, conservation and restoration of cultural and archeological heritage: research technologies and infrastructures for the science of cultural heritage, Mexico City, 02-03/02/2016. Invited lecture.
- Baglioni, P. Italian National Conference on Materials Science and Technology, Catania, 12-16/12/2016. Invited lecture.
- 16. Baglioni, P. IV International workshop on research, conservation and valorization of architectural monuments: preservation of built heritage, Lima (Peru), 04-06/05/2016. Invited lecture.
- 17. Baglioni, P. La fisica incontra la città Phisics meets the city, Università degli Studi Roma Tre, 9th March 2016. Public invited lecture.
- Baglioni, P. Nano and advanced materials for cultural heritage, Bruxelles (Belgio), 24/05/2016. Invited lecture.
- 19. Baglioni, P. Nanoinnovation 2016, Rome, 20-23/09/2016. Invited lecture.
- 20. Baglioni, P. Nanotechitaly, Roma, 21/09/2016. Invited lecture.
- Baglioni, P. Nanotechnology applied to conservation and restoration, Pinacoteca de Sao Paulo, Brasil, 07/04/2016. Invited lecture.
- 22. Baglioni, P. Our Past, your Future, Venezia, 29-30/10/2016. Invited lecture.
- Baglioni, P. Second Riches Polymer Seminar New horizons for cultural heritage, Bruxelles (Belgio), 23/05/2016. Invited lecture.
- Baglioni, P. Third Riches Polymer Seminar Networking session of EC-funded projects, Berlin, 22/11/2016. Invited lecture.
- 25. Baglioni, P.; Pensabene, L. 'Sette'-Magazine del Corriere della sera, 02/09/2016. "Il Picasso che non ti aspetti, ritrovato sotto una mano di bianco". Invited article and Youtube.
- Baratto, M.C.; Al Khatib, M.; Harir, M; Pogni, R.; Basosi, R. Xth EFEPR Conference, Torino (Italy), 04-08/09/2016. Poster.
- 27. Basosi, R. Congresso ATI 15/09/2016. Plenary lecture.
- 28. Basosi, R. University of Beni Mellal (Morocco), 19/10/2016. Plenary lecture.
- 29. Basosi, R. University of Teheran 30/08/2016. Plenary lecture.
- 30. Berretti, E.; Di Benedetto, F.; Cioffi, N.; Capolupo, F.; Lavacchi, A.; Picca, R.A.; Comparini, A.; Passaponti, M.; Innocenti, M. Enerchem-1, Firenze, 18-20/02/2016. Poster.
- 31. Berti, D. 30th Conference of the European Colloid and Interaface Society, Rome, September 2016. Invited lecture.
- Berti, D. Nanostructured materials meet lipid bilayer membranes: a colloidal perspective, Università di Tor Vergata, Dipartimento di Chimica, Roma (Italia), Aprile 2016. Invited presentation.
- Bonechi, C.; Tamasi, G.; Donati, A.; Magnani, A Rossi, C. 13th Edition Emory-Unisi Summer School, Chemistry for Life and Environment, Siena, 27/05/2016-04/07/2016. Poster.



- Byelyakova, A.; Tamasi, G.; Rossi, C. 13th Edition Emory-Unisi Summer School, Chemistry for Life and Environment, Siena, 27/05/2016-04/07/2016. Poster.
- Caminati, G. 16th International Conference on Organized Molecular Films (ICOMF16)-LB16, Helsinki (Finland), 25-29/07/2016. Oral presentation.
- Carretti, E.; Scarano, S.; Dei, L.; Minunni, M.; Baglioni, P. 251 American Chemical Society (ACS) Spring meeting, San Diego, CA, USA, 13-17/03/2016. Oral presentation.
- Casiello, M.; Sikorski, W.; Cotugno, P.; Monopoli, A.; Ciminale, F.; Picca, R.; Cioffi, N.; Bellebuono, L.; Irrera, A.; Trusso, S.; Lo Faro, M.J.; Trzeciak, A.M.; Nacci, A. 12th Congress of the Interdivisional Group of Organometallic Chemistry Genoa, 05-08/06/2016. Poster.
- Chaudhary, A.L.; Milanese, C.; Girella, A.; Bergemann, N.; Pistidda, C.; Klassen, T.; Dornheim, M. International Symposium on Metal – Hydrogen Systems MH 2016, Interlaken Switzerland, 07-12/08/2016. Oral presentation.
- Cioffi, N. N&N 2016 Nanoscience & Nanotechnology INFN Meeting 2016, INFN national laboratories, Frascati-Rome, 26-29/09/2016. Plenary lecture.
- Cofrancesco, P.; Milanese, C.; Trojsi, G.; Girella, A.; Valsecchi, G.; Bombeccari, M.; Frisetti A., XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Oral presentation.
- 41. Cuomo, F.; Ceglie, A.; Caltagirone, C.; Murgia, S.; Lopez, F. 30th Conference of The European Colloid and Interface Society (ECIS), Rome (Italy), 04-09/09/2016. Poster.
- Dallai, L.; Volpi. V.; Donati. A. CAA 2016 The 44rd Computer Applications and Quantitative Methods in Archaeology 'Exploring Ocean's of data' Conference, Oslo, 29/03/2016-02/04/2016. Poster.
- De Luca, A.; Giaccherini, A.; Comparini, A.; Pasquini, B.; Picca, R.A.; Cioffi, N.; Piciollo, E.; Furlanetto, S.; Di Benedetto, F.; Innocenti, M. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Messina), 18-22/09/2016. Poster.
- De Santis, A; Emendato, A; Russo Krauss, I; Picone, D; D'Errico, G; Pauanno, L. 6th EuCheMS Chemistry Congress, Seville (Spain), 11-15/09/16. Oral presentation.
- De Santis, A; Russo Krauss, I; Marasco, D; D'Errico, G. XLIV Congresso della Divisione di Chimica Fisica della Società Chimica Italiana. Napoli (Italy), 20-23/09/2016. Poster.
- Dilonardo, E.; Penza, M.; Alvisi, M.; Cassano, G.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium X. Poster.
- Dilonardo, E.; Penza, M.; Alvisi, M.; Rossi, R.; Cassano, G.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium X. Oral communication.
- Ditaranto, N.; Casiello, M.; Nacci, A.; Palmisano, F.; Sabbatini, L.; Torsi, L.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Messina), 18-22/09/2016. Invited oral communication.
- Donati, A. Congresso I paesaggi dell'allume: archeologia della produzione ed economia di rete, Roma-Siena, 09-11/05/2016. Oral presentation.
- 50. Ferraro, G.; Fratini, E.; Rausa, R.; Baglioni P. ECIS Conference, Roma (Italy), 05-09/09/2016. Oral presentation.
- Ferraro, G.; Fratini, E.; Rausa, R.; Baglioni P. EMRS Fall Meeting, Warsaw (Poland), 19-22/09/2016. Poster.
- Franchini, C.; Cavalluzzi, M.M.; Gualdani, R.; Moncelli, M.R.; Lentini, G. XXIV National Meeting in Medicinal Chemistry, Perugia (Italy), 11-14/09/2016. Poster.
- Gaboardi, M.; Milanese, C.; Magnani, G.; Mauron, P.; Duyker, S.; Peterson, V.K.; Saldan, I.; Pontiroli, D.; Galinetto, P.; Riccò, M. 10th International Symposium Hydrogen & Energy, Sendai (Japan), 21-26/02/2016. Oral presentation.
- 54. Galinetto P.; Albini, B.; Mozzati, M.C.; Bini, M.; Tondo, C.; Capsoni, D. CNISM-Materials 2016, Catania (Italia) 12-16/12/2016. Poster.
- Giaccherini, A.; Giurlani, W.; Pasquini, B.; Capolupo, F.; Picca, R.A.; Felici, R.; Carlà, F.; Cioffi, N.; Furlanetto, S.; Lavacchi, A.; Di Benedetto, F.; Innocenti, M. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Italy), 18-22/09/2016. Oral communication.
- Giaccherini, A.; Picca, R.A.; Sportelli, M.C.; Capolupo, F.; Montegrossi, G.; Cioffi, N.; Felici, R.; Carlà, F.; Lavacchi, A.; Di Benedetto, F.; Innocenti, M. Enerchem-1, Firenze (Italy), 18-20/02/2016. Poster.
- 57. Giorgi, R. II Simposio Internacional Andrew W. Mellon: El esplendor del Pórtico de la Gloria: conservación, policromía y la transfiguración de la material, 07-08/07/2016. Oral presentation.
- Giorgi, R. International Winter School Molecules@Surfaces, Societa' Chimica Italiana, 31/01-05/2/2016, Villaggio Olimpico di Bardonecchia. Oral presentation.
- Giorgi, R. Meeting SSH 2016 Net4Society SSH in H2020 Societal Challenge 6 and integration in other challenges, Bruxelles, 05/07/2016. Oral presentation.

- Giorgi, R.; Baglioni, M.; Shashoua, Y.; Brajer, I.; Baglioni, P. XVI Congresso nazionale di Chimica dell'Ambiente e dei Beni Culturali - Dall'emergenza alla salvaguardia: la chimica per un nuovo modello di sviluppo, Lecce, 26-29/06/2016. Oral presentation.
- 61. Gualdani, R. Regional Biophysics Conference RBC2016, Trieste (Italy), 25-28/08/2016. Invited talk.
- Gualdani, R.; Cavalluzzi, M.M.; Lentini, G. XXIII Congresso Nazionale SIBPA 2016, Cortona (Italy) 18-21/09/2016. Poster.
- Gualdani, R.; Guerrini, A.; Fantechi, E.; Sangregorio, C.; Moncelli, M.R. 60th Biophysical Meeting, Los Angeles (USA), 27/02/2016-02/03/2016. Poster.
- 64. Harir, M.; Baratto, M.C.; Basosi, R.; Pogni, R. Oxizymes 2016, Wageningen, 03-06/07/2016. Poster.
- Innocenti, M.; Di Benedetto, F.; Giaccherini, A.; Guerri, A.; Lavacchi, A.; Comparini, A.; Miller, H.; Carlà, F.; Felici, R.; Picca, R.A.; Cioffi, N.; Vizza, F. ECM6: 6th International symposium on Energy Challenges and Mechanics, Inverness (Scotland), 14-18/08/2016. Invited oral communication.
- Innocenti, M.; Giaccherini, A.; Di Benedetto, F.; Lavacchi, A.; Miller, H.A.; Cioffi, N.; Picca, R.A.; Vizza, F. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Italy), 18-22/09/2016. Oral communication.
- 67. Licciardello, A. Workshop & reunion des utilisateurs francophones ToF-SIMS, Mons, 09-10/03/2016. "SIMS and chemistry: from surface engineering to sputtering of polymers". Invited oral presentation.
- Lisi, S.; Ravelet, C.; Scarano, S.; M. Minunni, M.; Peyrin, E. Aptamers in Bordeaux, Bordeaux (France), June 2016. Poster.
- 69. Lisi, S.; Ravelet, C.; Scarano, S.; Minunni, M.; Peyrin, E. Biosensors 2016, Gothenburg (Sweden), 25-27/05/2016. Poster.
- Lisi, S.; Scarano, S.; Fedeli, S.; Cicchi, S.; Ravelet, C.; Peyrin, E.; Minunni, M. Bioanalitica 2016, giornata scientifica "Chimica bioanalitica e nanotecnologie", Bologna, 04/07/2016. Oral presentation.
- 71. Lisi, S.; Scarano, S.; Ravelet, C.; Peyrin, E.; Minunni, M. Biosensors 2016, 25-27/05/2016, Gothenburg (Sweden). Poster.
- Luchini A.; Gerelli Y.; Fragneto G.; Nylander T.; Paduano L. VI EuCheMS Chemistry Congress, Seville (Spain), 11-15/09/2016. Oral presentation.
- Luchini, A.; Gerelli, Y.; Fragneto, G.; Nylander, T.; Paduano, L. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli, 20-23/09/16. Poster presentation.
- Maranghi, S.; Parisi, M.L; Sinicropi, A.; Basosi, R. 1° Congress of the Interdivisional Group of Chemistry for Renewable Energy of the Italian Chemical Society (ENERCHEM-1), Florence (FI), 18-20/02/2016. Poster.
- Maranghi, S.; Parisi, M.L.; Basosi, R. IX Convegno della Rete Italiana LCA, Ravenna (RA), 23-24/06/2016. Poster.
- Marletta, G. 8th International School on Organic Electronics: Nano-Organics and devices, Paris, France, 04-08/07/2016. Invited lecture.
- 77. Marletta, G. Symposium PM1 Fall Meeting MRS, Boston 28/11-02/12/2016. Invited lecture.
- Martina, M.R.; Baglioni, P.; Caminati, G. 16th International Conference on Organized Molecular Films (ICOMF16)-LB16, Helsinki (Finland), 25-29/07/2016. Oral presentation.
- 79. Mavelli, F. COMSOL Conference, Munich, Germany, 12-14/10/2016. Oral presentation.
- Mavelli, F. International Workshop on Synthetic Approach to Origin of Life, Glasgow University, 29-30/09/2016. Invited oral presentation.
- 81. Mavelli, F. Wivace-Bionam 2016, Università di Salerno, Italy, 4-7/10/2016. Oral presentation.
- Messina, G.M.L.; Marletta, G. E-MRS Spring Meeting, Lille (France), 02-06/05/2016. Oral presentation.
- Messina, G.M.L.; Marletta, G. PEPMAT Peptide Materials for biomedicine and Nanotechnology, Barcelona (Spain), 13-17/03/2016. Invited lecture.
- Messina, G.M.L.; Marletta, G. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli, Italy, 20-23/09/2016. Oral presentation.
- Messina, G.M.L.; Marletta, G.; De Zotti, M.; Formaggio, F. Materials.IT, Catania, Italy, 19-23/12/2016. Oral presentation.
- Milanese, C.; Girella, A.; Valsecchi, G.; Bombeccari, M.; Cofrancesco, P.; Marini, A.; Rueda Noriega, M.; Sanz-Moral, L.M.; Martin, A.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Oral presentation.
- Milanese, C.; Girella, A.; Valsecchi, G.; Bombeccari, M.; Cofrancesco, P.; Marini, A.; Gaboardi, M.; Pontiroli, D.; Magnani, G.; Riccò, M. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Poster presentation.
- Milanese, C.; Girella, A.; Valsecchi, G.; Marini, A.; Gaboardi, M.; Pontiroli, D.; Magnani, G.; Riccò, M. E-MRS Fall Meeting 2016, Varsaw, Poland, 19-22/09/2016. Oral presentation.
- Milanese, C.; Girella, A.; Valsecchi, G.; Saldan, I.; Gaboardi, M.; Pontiroli, D., Magnani, G.; Riccò, M.; Marini, A. International Symposium on Metal – Hydrogen Systems, MH 2016, Interlaken, Switzerland, 07-12/08/2016. Oral presentation.

- Milanese, C.; Pontiroli, D.; D'Alessio, D.; Gaboardi, M.; Magnani, G.; Duyker, S.K.; Peterson, V.K.; Sharma, N.; Riccò, M. International Symposium on Metal – Hydrogen Systems MH 2016, Interlaken Switzerland, 07-12/08/2016. Poster presentation.
- Milanese, C.; Saldan, I.; Girella, A.; Valsecchi, G.; Cofrancesco, P.; Marini, A.; Rueda Noriega, M.; Sanz-Moral, L.M.; Martin, A.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M. E-MRS Fall Meeting 2016, Varsaw, Poland, 19-22/09/2016. Oral presentation.
- 92. Milanese, C.; Saldan, I.;, Girella, A., Valsecchi, G.; Cabrini, E.; Pallavicini, P.; Galinetto, P.; Rueda Noriega, M.; Martin, A.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M.; Marini, A. 10th International Symposium Hydrogen & Energy, Sendai, Japan, 21-26/02/2016. Oral presentation.
- Mozzachiodi, S.; Cardelli, L.; Stano, P.; Altamura, E.; Mavelli, F.; Marangoni, R. 13th Annual Meeting of the Bioinformatics Italian Society (BIT 2016), Università di Salerno (Italy), 15-17/06/2016. Poster.
- Murgia, S. 2nd International Symposium on Nanoparticles/Nanomaterials and Applications, Caparica, Portogallo, 18-21/01/2016. Keynote lecture.
- Murgia, S. Engineering Conference International, Hernstein, Austria, 10-14/07/2016. Invited speaker.
 Murgia, S.; Meli, V.; Caltagirone, C.; Falchi, A.M.; Lippolis, V.; Hyde, S.T.; Monduzzi, M.; Obiols-
- Rabasa, M.; Rosa, A.; Schmidt, J.; Talmon, Y. 30th ECIS Conference, Rome, 04-09/09/2016. Poster.
- 97. Murgia. S. XLIV Congresso Divisione Chimica Fisica, Napoli, 20-23/09/2016. Oral presentation.
- Nairi, V.; Salis, A.; Fanti, M; Medda, L; Cugia, F.; Piludu, M; Sogos, V.; Monduzzi M. 30th ECIS Conference, Roma (Italy), 04-09/09/2016. Poster.
- Perfetti, M.; D'Errico, G.; Paduano L. 6th European Association of Chemical and Materials Societies (EuCheMs) International Congress Conference of the European Colloid and Interface Society, Siviglia (Spain), 11-15/09/2016. Poster.
- Perfetti, M.; D'Errico, G.; Paduano L. XLIV Congresso della Divisione di Chimica Fisica della Società Chimica Italiana. Napoli (Italy), 20-23/09/2016. Oral presentation.
- Perfetti, M.; Heenan, R.K.; D'Errico, G.; Paduano L. 30th Conference of the European Colloid and Interface Society, Roma (Italy), 04-09/09/2016. Poster.
- Pica, A.; Russo Krauss, I.; Parente, V.; Sica, F. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli. Napoli (Italy), 20-23/09/16. Poster.
- Picca, R.A.; Cinotti, S.; Giaccherini, A.; Sportelli, M.C.; Di Benedetto, F.; Innocenti, M.; Cioffi, N. Enerchem-1, Firenze, 18-20/02/2016. Oral communication.
- 104. Picca, R.A.; Giaccherini, A.; Di Benedetto, F.; Innocenti, M.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Messina), 18-22/09/2016. Oral communication.
- Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Sportelli, M.C.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. EMN Croatia Meeting 2016 Dubrovnik, 04-07/05/2016. Invited communication.
- 106. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Italy), 18-22/09/2016. Oral communication.
- 107. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, Sportelli, M.C.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium L. Poster.
- Picca, R.A.; Paladini, F.; Sportelli, M.C.; Pollini, M.; Giannossa, L.C.; Di Franco, C.; Mangone, A.; Valentini, A.; Sannino, A.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium S. Oral communication.
- Picca, R.A.; Sportelli, M.C.; Ditaranto, N.; Giannossa, C.; Mangone, A.; Di Franco, C.; Paladini, F.; Pollini, M.; Sannino, A.; Tütüncü, E.; Kranz, C.; Mizaikoff, B.; Valentini, M.; Valentini, A.; Cioffi, N. EMN Energy Materials Nanotechnology, Cancun, Mexico, 04-09/06/2016. Invited oral communication.
- Picca, R.A.; Sportelli, M.C.; Lopetuso, R.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium AA. Poster.
- Picca, R.A.; Sportelli, M.C.; Lopetuso, R.; Villone, V.; Cioffi, N. 12th Congress of the Interdivisional Group of Organometallic Chemistry, Genoa, 05-08/06/2016. Poster.
- Picca, R.A.; Sportelli, M.C.; Luciano, A.; Manoli, K.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. Orbitaly 2016 Santa Cesarea, Lecce (Italy) 26-28/10/2016. Invited oral communication.
- Picca, R.A.; Sportelli, M.C.; Quarto, R.; Ditaranto, N.; Valentini, A.; Cioffi, N. EMRS2016 Spring Meeting, Lille (France), 01-06/05/2016, Symposium Q. Poster.
- Picca, R.A.; Sportelli, M.C.; Quarto, R.; Valentini, A.; Cioffi, N. 12th Congress of the Interdivisional Group of Organometallic Chemistry Genoa, 05-08/06/2016. Poster.
- Picca, R.A.; Sportelli, M.C.; Villone, V.; Lopetuso, R.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Messina), 18-22/09/2016. Poster.
- 116. Pitzalis, F.; Salis, A.; Monduzzi, M. 30th ECIS Conference, Roma (Italy), 04-09/09/2016. Poster.

- 117. Pogni, R. Emory@Unisi, Siena, 21/06/2016. Invited lecture.
- Pontiroli, D.; D'Alessio, D.; Gaboardi, M.; Magnani, G.; Riccò, G.; Milanese, C.; Duyker, S.G.; Peterson, V.K.; Sharma, N. E-MRS Fall Meeting 2016, Warsaw (Poland), 19-22/09/2016. Oral presentation.
- 119. Pontiroli, D.; Gaboardi, M.; Magnani, G.; Aramini, M.; Riccò, M.; Duyker, S.G.; Peterson, V.K.; Mauron, P.; Girella, A.; Milanese, C. Tematic Meeting "Materials for Energy", Roma, Università La Sapienza (Italy), 09/09/2016. Oral presentation.
- Pontiroli, D.; Magnani, G.; Gaboardi, M.; Riccò, M.; Pramudita, J.C.; Sharma, N.; Milanese, C. 10th International Symposium Hydrogen & Energy, Sendai (Japan), 21-26/02/2016. Oral presentation.
- 121. Riccardi, C.; Musumeci, D.; Morvan, F.; Meyer, A.; Vasseur, J.J.; Russo Krauss, I.; Paduano, L., Montesarchio, D. 22th International Round Table on Nucleosides, Nucleotides and Nucleic Acids, Paris (France), 18-22/07/2016. Poster.
- Ridi, F.; Tonelli, M.; Resta, C.; Baglioni, P. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli, 20-23/09/2016. Poster.
- 123. Rossi, C.O.; Caputo, P.; Calandra, P.; Mezzi, A.; Teltayev, B; Angelico, R. 30th Conference of The European Colloid and Interface Society (ECIS), Rome (Italy), 04-09/09/2016. Poster.
- Rueda Noriega, M.; Sanz-Moral, L.M.; Saldan, I.; Girella, A.; Milanese, C.; Martín, A. International Symposium on Metal – Hydrogen Systems MH 2016, Interlaken (Switzerland), 07-12/08/2016. Oral presentation.
- Russo Krauss, I.; Napolitano, V.; Petraccone, L.; Mattia, C.A.; Sica, F. XLIV Congresso della Divisione di Chimica Fisica della SCI. Napoli (Italy), 20-23/09/16. Poster.
- 126. Russo Krauss, I.; Riccardi, C.; Montesarchio, D.; D'Errico, G.; Paduano, L. 30th Conference of the European Colloid and Interface Society, Roma (Italy), 05-09/09/16. Oral presentation
- Salis, A.; Cugia, F.; Sedda, S.; Pitzalis, F.; Monduzzi, M. 30th ECIS Conference, Roma (Italy), 04-09/09/2016. Oral presentation.
- Sarzi Amadè, N.; Sanna, S.; Carretta, P.; Riccò, M.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Milanese, C.; Girella, A. International Symposium on Metal – Hydrogen Systems MH 2016, Interlaken Switzerland, 07-12/08/2016. Oral presentation.
- Scarano, S.; Berlangieri, C.; Carretti, E.; Dei, L.; Baglioni, P.; Minunni M. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Giardini Naxos (ME), 18-22/09/2016. Poster.
- Scarano, S.; Bonini, M.; Manera, M.G.; Colombelli, A.; Rella, R.; Minunni M. Plasmonica 2016, Genova, 14-16/09/2016. Poster.
- Scarano, S.; Bonini, M.; Manera, M.G.; Rella, R.; Minunni, M. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Giardini Naxos (Italy), 18-22/09/2016. Oral presentation.
- 132. Scarano, S.; Carretti, E.; Baglioni, P.; Dei, L.; Minunni, M. Biosensors 2016, Gothenburg (Sweden), 25-27/05/2016. Poster.
- Scarano, S.; Minunni, M. "Molecular diagnostic by optical based sensing", Warsaw (Polonia), 12-14/09/2016. Invited lecture.
- 134. Scarano, S.; Minunni, M. Acoustic and electrochemical methods in the study of affinity interactions at surfaces, AEMIS 2016, Bratislava (Slovakia), 20/06/2016. Oral presentation.
- Scarano, S.; Minunni, M. Bioelectrochemistry and more...2016, Wiener Neustadt (Austria), 13-14/060/2016. Plenary invited presentation.
- Sinicropi, A.; Parisi, M.L.; Basosi, R. XLIV Congresso della Divisione di Chimica Fisica, Napoli, 20-23/09/2016. Poster.
- 137. Sinicropi, A.; Parisi, M.L.; Reginato, G.; Zani, L.; Calamante, M.; Mordini, A.; Basosi, R.; Taddei, M. 1° Congress of the Interdivisional Group of Chemistry for Renewable Energy of the Italian Chemical Society (ENERCHEM-1), Florence (Italy), 18-20/02/2016. Poster.
- Smeazzetto, S.; Young, H.S.; Trieber, C.A.; Moncelli M.R.; Tadini-Buoninsegni, F. 60th Biophysical Meeting, Los Angeles (USA), 27/02/2016-02/03/2016. Poster.
- 139. Spinelli, D.; Baratto, M.C.; Basosi, R.; Pogni, R. Oxizymes 2016, Wageningen, 03-06/07/2016. Poster.
- Sportelli, M.C.; Ancona, A.; Picca, R.A.; Izzi, M.; Di Maria, A.; Volpe, A.; Lugarà, P.M.; Cioffi, N. 12th Congress of the Interdivisional Group of Organometallic Chemistry Genoa, 05-08/06/2016. Oral communication.
- 141. Sportelli, M.C.; Ancona, A.; Picca, R.A.; Volpe, A.; Lugarà, P.M.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Italy), 18-22/09/2016. Oral communication.
- Sportelli, M.C.; Tütüncü, E.; Picca, R.A.; Valentini, M.; Valentini, A.; Kranz, C.; Mizaikoff, B.; Cioffi, N. ISA2016 Matera, 29/05/2016-01/06/2016. Oral communication.
- Sportelli, M.C.; Tütüncü, E.; Picca, R.A.; Valentini, M.; Valentini, A.; Kranz, C.; Mizaikoff, B.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium Q. Oral



communication.

- 144. Strambini, L.M.; Longo, A.; Scarano, S.; Prescimone, T.; Palchetti, I.; Minunni, M.; Giannessi, D.; Barillaro, G. Terzo Convegno Nazionale Sensori, Roma, 23-25/02/2016. Oral presentation.
- Tadini-Buoninsegni, F.; Smeazzetto, S.; Moncelli, M.R.; Trieber, C.A.; Young, H.S. XXIII Congresso Nazionale SIBPA 2016, Cortona (Italy) 18-21/09/2016. Oral presentation.
- Tamasi, G.; Bonechi, C.; Leone, G.; Donati, A.; Magnani, A.; Rossi, C. 13th Edition Emory-Unisi Summer School, Chemistry for Life and Environment, Siena, 27/05/2016-04/07/2016. Poster.
- Tonelli, M.; Resta, C.; Ridi, F.; Baglioni, P. 6th EuCheMS Chemistry Congress, Sevilla (Spain), 12-16/09/2016. Poster.
- Tonelli, M.; Ridi, F; Borsacchi, S.; Martini, F.; Calucci, L.; Geppi, M. 30th Conference of the European Colloid and Interface Society, Roma, 04-09/09/2016. Poster.
- 149. Tonelli, M.; Ridi, F.; Borsacchi, S.; Martini, F.; Calucci, L.; Fratini, E.; Geppi, M.; Baglioni, P. 4th International Workshop on: Mechanisms and Modelling of Waste /Cement Interactions, Structural characterization of magnesium silicate hydrate: towards the design of eco-sustainable cements, 22-25/05/2016. Oral presentation.
- 150. Tonelli, M.; Ridi, F.; Borsacchi, S.; Martini, F.; Calucci, L.; Fratini, E.; Geppi, M.; Baglioni, P. 4th International Workshop on: Mechanisms and Modelling of Waste /Cement Interactions, Structural characterization of magnesium silicate hydrate: towards the design of eco-sustainable cements, 22-25/05/2016. Poster.
- 151. Tovar Rodríguez, J.; Donato Moreno, J. E.; Galindo Esquivel, I.R.; Fratini, E.; Baglioni, P. Merck Young Chemists Symposium, MYCS 2016, Rimini (IT), 25-27/10/2016. Poster.
- Tovar Rodríguez, J.; González Rivera, J.; Ferrari, C.; Longo, I; Fratini, E.; Baglioni, P. European Materials Research Society, EMRS Fall Meeting 2016, Warsaw (Poland), 19-22/09/2016. Oral presentation.
- 153. Troisi, R.; Russo Krauss, I.; Napolitano, V.; Sica, F. XLIV Congresso della Divisione di Chimica Fisica della SCI. Napoli (Italy), 20-23/09/16. Poster presentation.
- Tuccitto, N.; Giamblanco, N.; Zappalà, G.; Licciardello, A.; Marletta, A. EMRS-Spring Meeting Lille (France), 2016. Oral presentation.
- 155. Tuccitto, N.; Marletta, G. Materials.IT, Catania (Italy), 19-23/12/2016. Oral presentation.
- Tuccitto, N.; Sfuncia, G.; Marletta, G. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Oral presentation.
- 157. Tuccitto, N.; Vitale, S.; Zappalà, G.; Ronconi, F.; Licciardello, A. EMRS-Fall Meeting, Warsaw (Poland), 2016. Poster.
- Tuccitto, N.; Zappalà, G.; Vitale, S.; Marletta, G.; Licciardello, A. EMRS-Fall Meeting, Warsaw (Poland), 2016. Invited keynote.
- 159. Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A.; Licciardello, A. SIMS Europe 2016, Münster (Germany), 18-20/09/2016. Oral presentation.
- Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A.; Licciardello, A. SIMS Europe 2016, Münster (Germany), 18-20/09/2016. Poster.
- Vitale, S.; Zappalà, G.; Santoni, M.P.; Tuccitto, N.; Hanan, G.; Campagna, S.; Licciardello, A. SIMS Europe 2016, Münster, Germany, 18-20/09/2016. Oral presentation.
- 162. Vitiello, G.; Silvestri, B.; Zanfardino, A.; Costantini, A.; Varcamonti, M.; D'Errico, G.; Branda, F.; Pezzella, A.; Luciani, G. XLIV Congresso Divisione Chimica-Fisica, Società Chimica Italiana (SCI), Napoli (Italy), 20-23/09/2016. Oral presentation.
- Volpi, V; Donati, A; Dallai, L. Conference Precious metal in the medieval mediterranean, Aix-en-Provence (France), 06-08/10/2016. Oral presentation.
- Weththimuni, M.L.; Capsoni, D.; Milenese, C.; Licchelli, M.; Malagodi, M. INART 2nd International Conference on Innovation in Art Research and Technology, Ghent (Belgium), 21-25/03/2016. Oral presentation.
- 165. Altamura, E.; Cazzolla, F.; Palazzo, G.; Stano, P.; Mavelli, F. Wivace 2015 Italian Workshop of artificial Life and Evolutionary Computing, Bari (Italy), 22-24/09/2015. Poster.
- Altamura, E.; Regina, G.; Stano, P.; Mavelli, F. Wivace 2015 Italian Workshop of artificial Life and Evolutionary Computing, Bari (Italy), 22-24/09/2015. Poster.
- Altamura, E.; Stano, P.; Mavelli, F. Congresso Nazionale della Società Italiana di FotoBiologia (SIFB 2015), Università degli Studi di Bari (Italy), 11-13/06/2015. Oral presentation.
- Altamura, E.; Stano, P.; Mavelli, F. Syschem 2015, Abdij Rolduc (the Netherlands), 19-22/05/2015. Oral presentation.
- Altamura, E.; Stano, P.; Mavelli, F.; Milano, F.; Tangorra, R.R.; Omar, O.H.; Farinola, G.M.; Mavelli, F. Wivace 2015 - Italian Workshop of artificial Life and Evolutionary Computing, Bari (Italy), 22-24/09/2015. Oral presentation.
- 170. Altamura, E.; Vucojevic, V.; Mavelli, F. Working group meeting COST Action CM1304 -Biomimetic compartmentalized chemical systems, Università di Bari (Italy), 25-26/09/2015. "Characterizing giant vesicles composition by fluorescence correlation spectroscopy". Oral

presentation.

- 171. Ancona, A.; Picca, R.A.; Di Maria, A.; Řiháková, L.; Volpe, A.; Sportelli, M-C; Lugarà, P.M.; Cioffi, N. 2015 MRS Fall Meeting & Exhibit, 29/11-04/12/2015, Boston, Massachusetts. Poster.
- 172. Ancona, A.; Picca, R.A.; Di Maria, A.; Řiháková, L.; Volpe, A.; Sportelli, M.C.; Lugarà, P.M.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Poster.
- 173. Angelico, R.; Ceglie, A.; Sacco, P.; Ripoli, M.; Mangia, A. School of Nanomedicine, organizzata dal Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali (INSTM – Firenze) e dall'Istituto di Cristallografia CNR-IC, Bari (Italy), 02-04/12/2015. Poster.
- Baglioni, M.; Bartoletti, A.; Bozec, L.; Chelazzi, D.; Giorgi, R.; Odlyha, M.; Pianorsi, D.; Baglioni,
 P. E-MRS European Materials Research Society, Spring Meeting 2015, Lille (France), 11-13/05/2015. Oral presentation.
- 175. Baglioni, P. 1st European Conference on Physical and Theoretical Chemistry, Catania, 15-18/09/2015. Plenary lecture.
- Baglioni, P. 2015 Materials Research Society Fall Meeting & Exibit, Boston (USA), 30/11-04/12/2015. Invited lecture.
- Baglioni, P. Fifth International Colloids Conference: Colloid and Interface Sciences for a Brighter Future, Amsterdam (Olanda), 21-24/06/2015. Invited lecture.
- 178. Baglioni, P. Conservation of cultural heritage: challenges and reviews, Atene (Grecia), 25-29/05/2015. Invited lecture.
- 179. Baglioni, P. EuroNanoForum 2015, Riga (Lettonia), 10-12/06/2015. Invited lecture.
- Baglioni, P. Future and Current Use of Neutron Spin-Echo Spectroscopy in Condensed Matter Research Workshop, Oak Ridge, USA, 12-16/05/2015. Invited lecture.
- 181. Baglioni, P. International workshop on the application of nano-lime for consolidation of weathered stones, Bath University, UK, 24th September 2015. Invited lecture.
- 182. Baglioni, P. Jülich Soft Matter Days 2015, Bad Honnef (Germany), 10-13/11/2015. Invited lecture.
- 183. Baglioni, P. NanotechItaly 2015, Bologna, 25-26/11/2015. Invited lecture.
- Baglioni, P. Nanotechnologies for cultural conservation: current trends and practices, IDEAL Center for Innovation of Lafayette College, Allentow, Pennsylvania (USA), 30-31/10/2015. Plenary lecture.
- 185. Baglioni, P. National Congress of Italian Physical Society, Rome, Italy, 25th September 2015. Invited lecture.
- Baglioni, P. Oorgandagarna 2015, Wisby Strand Sweden, Stoccolma (Svezia), 15-17/06/2015. Invited lecture.
- Baglioni, P. RICHES Renewal, Innovation and Change Heritage and European Society, Bruxelles, 19th October 2015. Oral presentation.
- Baglioni, P. Science and Innovation for the study and conservation of works of art, Rio de Janeiro (Brazil), 4th December 2015. Invited lecture.
- Bardi, A.; Dallai, L.; Donati. A.; Volpi. V. CAA 2015 The 43rd Computer Applications and Quantitative Methods in Archaeology "Keep the revolution going" Conference, Siena, 30/03/2015-03/04/2015. Oral presentation.
- 190. Basosi, R. Biwaes, Stockholm, 04/05/2015. Plenary lecture.
- 191. Basosi, R. Jagellonian, University Krakow, 16/02/2015. Plenary lecture.
- 192. Bergemann, N.; Pistidda, C.; Karimi, F.; Gobetto, R.; Milanese, C.; Emmler, T.; Klassen, T.; Dornehim, M. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications". Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
- 193. Berretti, E.; Cinotti, S.; Picca, R.A.; Di Benedetto, F.; Cioffi, N.; De Luca, A.; Lavacchi, A.; Innocenti, M. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Poster.
- Berti, D. 15th Conference of the International Association of Colloid and Interface Scientists, Mainz (Germany), 24-29/05/2015. Invited keynote lecture.
- 195. Berti, D. 5th International Colloids Conference, Amsterdam, Netherlands, 21-24/06/2015. Invited keynote lecture.
- Berti, D. Jülich Centre for Neutron Science Workshop, Tutzing (Germany), 05-08/10/2015. Invited lecture.
- 197. Berti, D. Hybrid Soft Nanostructured Architectures: Structural, Functional and Biophysical Aspects, Università di Salerno (Italia), Marzo 2015. Invited presentation.
- Berti, D. Soft Matter for Biological Applications An Overview, CNR-ISMN, Bologna (Italia), Luglio 2015. Invited presentation.
- Bonechi, C.; Tamasi, G.; Donati, A.; Magnani, A.; Rossi, C. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
- Bonini, M.; Gelli, R.; Del Buffa, S.; Tempesti, P.; Ridi, F.; Baglioni, P. EMRS Spring meeting, Lille, Marzo 2015. Oral presentation.
- Borsacchi, S.; Martini, F.; Calucci, L.; Ridi, F.; Tonelli, M.; Fratini, E.; Baglioni, P. Geppi, M. XLIV National congress on magnetic resonance, Roma, 28-30/09/2015. Oral presentation.



- Borsacchi, S.; Martini, F.; Geppi, M.; Fratini, E.; Ridi, F.; Tonelli, M.; Calucci, L. 9th Field-Cycling NMR conference, Aberdeen, 27-30/07/2015. Oral presentation.
- 203. Busi, E.; Maranghi, S.; Corsi, L.; Basosi, R. International conference on Life Cycle Assessment as reference methodology for assessing supply chains and supporting global sustainability challenges, Stresa and Milano, 06-08/10/2015. Poster.
- 204. Calvano, C.D.; Picca, R.A.; Bonerba, E.; Ditaranto, N.; Pellegrini, T.; Tantillo, G.; Cioffi, N.; Palmisano, F. 4th MS Food Day, 07-09/10/2015, Foggia (Italy). Poster.
- Calvano, C.D.; Picca, R.A.; Bonerba, E.; Ditaranto, N.; Tantillo, G.; Cioffi, N.; Palmisano, F. XXV Congresso Nazionale di Chimica Analitica, Trieste, 13-17/09/2015. Poster.
- Caminati, G. 14th European Conference on Organized films ECOF-14, Genova (Italy), 29/06-02/07/2015. Oral presentation.
- 207. Capurso, G.; Bellosta von Colbe, J.M.; Gupta, N.; Yigit, D.; Pendolino, F.; Melnichuk, M.; Milanese, C.; Girella, A.; Taube, K.; Klassen, T.; Dornheim, M. Gordon Research Conference "Hydrogen Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications". Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
- Cofrancesco, P.; Frisetti, A.; Licchelli, M.; Milanese, C.; Trojsi, G. 1st International Conference on Metrology for Archaeology, Benevento (Italy), 22-23/10/2015. Oral presentation.
- Cugia, F.; Monduzzi, M.; Salis, A. 1st European Conference on Physical and Theoretical Chemistry Catania (Italy), 14-18/09/2015. Poster.
- Cuomo, F.; Lopez, F.; Ceglie, A.; Miguel, M.G.; Lindman, B. 15th Conference of the International Association of Colloid and Interface Scientists. Mainz (Germany), 24-29/05/2015. Oral presentation.
- 211. Cuomo, F.; Lopez, F.; Ceglie, A.; Miguel, M.G.; Lindman, B. 1st European Conference on Physical and Theoretical Chemistry and XLII annual meeting of the Physical Chemistry Division of SCI, Catania (Italy), 14-16/09/2015. Poster.
- 212. De Santis, A; Vitiello, G; D'Errico, G; Paduano, L. 1st European Conference on Physical and Theoretical Chemistry, Catania, 10-14/09/2015. Poster.
- Dilonardo, E.; Penza, M.; Alvisi, M.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Oral communication.
- Dilonardo, E.; Penza, M.; Alvisi, M.; Di Franco, C.; Suriano, D.; Palmisano, F.; Torsi, L.; Cioffi, N. MRS2015 Spring Meeting, San Francisco, CA, (USA), 21-25/04/2015. Poster.
- Dilonardo, E.; Penza, M.; Alvisi, M.; Difranco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. MRS2015 Spring Meeting, San Francisco, CA, (USA), 21-25/04/2015. Oral communication.
- Dilonardo, E.; Penza, M.; Alvisi, M.; Rossi, R.; Di Franco, C.; Torsi, L.; Cioffi, N. COST Action TD1105 EuNetAir 3rd International Workshop EuNetAir, Riga (Latvia), 26-27/03/2015. Oral communication.
- 217. Ditaranto, N.; Picca, R.A.; Sportelli, M.C.; Sabbatini, L.; Cioffi, N. 16th European Conference on Applications of Surface and Interface Analysis ECASIA'15, Granada (Spain) 28/09-01/10/2015. Oral communication.
- 218. Donati, A; Bardi, A.; Volpi, V.; Mencuccini, L.; Bianchi, G.;, Benvenuti, M.; Chiarantini, L.; Rossi, C.; Dallai, L. The 1st European Conference on Physical and Theoretical Chemistry and XLII Annual Meeting of the Physical Chemistry Division of SCI, Catania, 14-18/09/2015. Oral presentation.
- Giaccherini, A.; Cinotti, S.; Picca, R.A.; Carlà, F.; Montegrossi, G.; Capolupo, F.; Felici, R.; Di Benedetto, F.; Furlanetto, S.; Cioffi, N.; Lavacchi, A.; Innocenti, M. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Oral communication.
- 220. Giorgi, R. Conference at Lafayette College 2015 Easton, PA (USA), 02/11/2015. Oral presentation.
- Giorgi, R. Keynote at XV Congresso Nazionale Divisione Chimica dell'Ambiente e dei beni Culturali, Società Chimica Italiana, Bergamo, 14-18/06/2015. Oral presentation.
- 222. Giorgi, R. NanoItaly 2015, Roma University of Rome La Sapienza, 21-24/09/2015. Oral presentation.
- 223. Giorgi, R.; Poggi, G.; Mirabile, A.; Hui Ping, X.; Baglioni, P. E-MRS European Materials Research Society, Spring Meeting 2015, Lille (France), 11-13/05/2015. Oral presentation.
- Gualdani, R.; di Cesare Mannelli, L.; Francesconi, O.; Ghelardini, C.; Moncelli M.R.; Richichi, B.; Nativi, C. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
- Gualdani, R.; Guerrini, A.; Fantechi, E.; Moncelli, M.R.; Sangregorio, C. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
- Lamberti, I.; Scarano, S.; Esposito, C.L.; Antoccia, A.; Antonini, G.; Tanzarella, C.; De Franciscis, V.; Minunni, M. XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Trieste, 13-17/09/2015. Poster.
- 227. Lisi, S.; Scarano, S.; Ravelet, C.; Peyrin, E.; Minunni M. Biaoanalitica 2015, Firenze, 26/06/2015. Poster.
- 228. Lisi, S.; Scarano, S.; Ravelet, C.; Peyrin, E.; Minunni, M. XXV Congresso della Divisione di Chimica

Analitica della Società Chimica Italiana (SCI), Trieste, 13-17/09/2015. Poster.

- 229. Lisi, S.; Scarano, S.; Ravelet, C.; Peyrin, E.; Minunni, M. XXXIV Congresso Interregionale delle Sezioni Toscana, Umbria, Marche e Abruzzo della Società Chimica Italiana - TUMA 34, 23-25/09/2015. Oral presentation.
- 230. Lopez, F.; Venditti, F.; Ambrosone, L.; Cuomo, F.; Ceglie, A. Workshop "Chimica, Ambiente e Territorio" organizzato dalla Società Chimica Italiana, Sezione Campania, e dal Dipartimento di Scienze e Tecnologie Ambientali, Biologiche e Farmaceutiche della Seconda Università di Napoli. Caserta (Italy), 30/09/2015. Oral presentation.
- Lopez, F.; Venditti, F.; Cuomo, F.; Ceglie, A. 1st European Conference on Physical and Theoretical Chemistry and XLII annual meeting of the Physical Chemistry Division of SCI, Catania (Italy), 14-16/09/2015. Poster.
- Luchini, A.; Gerelli, Y.; Fragneto, G.; Paduano, L. XXVI Congresso Annuale SISN Italian Neutron Scattering Conference, Frascati-Roma, 01-03/07/2015. Oral presentation.
- Luci, G.; Vanni, M.; Minunni, M.; Intorre, L.; Meucci V. Atti Sisvet LXVIII. Vol. LXIX, Perugia, 16-18/06/2015. Poster.
- 234. Martini, F.; Calucci, L.; Geppi, M.; Fratini, E.; Ridi, F.; Tonelli, M.; Baglioni P.; Borsacchi S. GIDRM 2015, Roma, 28-30/09/2015. Poster and oral presentation.
- Martini, F.; Calucci, L.; Geppi, M.; Fratini, E.; Ridi, F.; Tonelli, M.; Baglioni, P.; Borsacchi, S. EUROMAR 2015, Praga, 05-10/07/2015. Oral presentation.
- Mavelli, F.; Altamura, E.; Stano, P. Working group meeting COST Action CM1304 Biomimetic compartmentalized chemical systems, Università di Bari (Italy), 25-26/09/2015. Oral presentation.
- 237. Mavelli, F.; Emiliano, A.; Stano, P. Syschem 2015, Abdij Rolduc, the Netherlands, 19-22/05/2015. Oral presentation.
- Meli, V.; Murgia, S.; Caltagirone, C.; Falchi, A.M.; Monduzzi, M. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
- Merlino, A.; Russo Krauss, I.; Caterino, M.; Vergara A. 29th Annual Symposium of The Protein Society, Barcelona (Spain), 22-25/07/2015. Poster.
- Messina, G.M.L. BioEl 2015 BioEl 2015 International Winterschool on Bioelectronics, Kirchberg in Tyrol (Austria), 28/02-07/03/2015. Poster.
- 241. Messina, G.M.L.; Karakeçili, A.; Yurtsever, M.; Gümüşderelioğlu, M.; Marletta, G. Euro Biomat, Weimar, Germany, 21-22/04/2015. Oral presentation.
- 242. Messina, G.M.L.; Marletta, G. E-MRS Spring Meeting, Lille, France, 11-15/05/2015. Oral presentation.
- 243. Messina, G.M.L.; Marletta, G. EuroPhysChem, Catania, Italy, 14-18/09/2015. Oral presentation.
- Milanese, C.; Girella, A.; Saldan, I.; Marini, A.; Gaboardi, M.; Pontiroli, D., Magnani, G.; Riccò, M. 1st European Conference on Physical and theoretical chemistry, Catania (Italy), 14-18/09/2015. Oral presentation.
- 245. Milanese, C.; Girella, A.; Saldan, I.; Rueda Noriega, M.; Martin, A.; Marini, A. 1st European Conference on Physical and theoretical chemistry, Catania, (Italy) 14-18/09/2015. Poster.
- Milanese, C.; Girella, A.; Saldan, I.; Valsecchi, G.; Gaboardi, M.; Pontiroli, D.; Magnani, G.; Riccò, M.; Marini, A. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications". Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
- Murgia, S.; Meli, V.; Falchi, A.M.; Nylander, T.; Schillén, K.; Monduzzi, M.; Talmon, Y. 5th International Colloids Conference, Amsterdam (The Netherlands), 21-24/06/2015. Poster.
- Picca, R.A.; Ditaranto, N.; Sportelli, M.C.; Pellegrini, T.; Valentini, A.; Cioffi, N. 2015 Materials Research Society Fall Meeting & Exhibit, 29/11-04/12/2015, Boston, Massachusetts. Poster.
- Picca, R.A.; Fazio, B.; Calvano, C.D.; Lo Faro, M.J.; Sportelli, M.C.; D'Andrea, C.; Irrera, A.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Poster.
- 250. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Sportelli, M.C.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. 2015 Materials Research Society Fall Meeting & Exhibit, 29/11-04/12/2015, Boston, Massachusetts. Poster.
- 251. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Sportelli, M.C.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. 4th MS Food Day, 07-09/10/2015, Foggia (Italy). Oral communication.
- Picca, R.A.; Manoli, K.; Sportelli, M.C.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. 2015 Materials Research Society Fall Meeting & Exhibit, 29/11-04/2015, Boston, Massachusetts. Oral communication.
- 253. Picca, R.A.; Paladini, F.; Sportelli, M.C.; Pollini, M.; Giannossa, L.C.; Di Franco, C.; Mangone, A.; Valentini, A.; Sannino, A.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Keynote.
- Picca, R.A.; Sportelli, M.C.; Calvano, C.D.; Ditaranto, N.; Cioffi, N. EMN Energy Materials Nanotechnology, Cancun (Mexico), 07-11/06/2015. Invited oral communication.


- Picca, R.A.; Sportelli, M.C.; Luciano, A.; Cioffi, N. Materials Research Society 2015 Spring Meeting, San Francisco, CA (USA), 21-25/04/2015. Poster.
- 256. Picca, R.A.; Sportelli, M.C.; Luciano, A.; Manoli, K.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. GEI Giornate dell'Elettrochimica Italiana 2015, Bertinoro, 20-24/09/2015. Oral communication.
- 257. Picca, R.A.; Sportelli, M.C.; Luciano, A.; Manoli, K.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. International Workshop on the Electrochemistry of Electroactive Materials WEEM – 2015 Bad Herrenalb (Germany), 31/05-05/06/2015. Invited oral communication.
- Picca, R.A.; Sportelli, M.C.; Luciano, A.; Manoli, K.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. MRS2015 Spring Meeting, San Francisco, CA (USA), 21-25/04/2015. Poster.
- Pistidda, C.; Hardian, R.; Bergemann, N.; Horstmann, C.; Milanese, C.; Girella, A.; Capurso, G.; Bellosta von Colbe, J.M., Chaudhary, A.L.; Metz, O.; Gupta, N.; Taube, K.; Klassen, T.; Dornheim, M. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications", Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
- Pitzalis, F.; Cugia, F.; Salis, A.; Carboni, D.; Malfatti, L.; Innocenzi, P.; Monduzzi, M. 1st European Conference on Physical and Theoretical Chemistry, Catania (Italy), 14-18/09/2015. Poster.
- Pogni, R. GIRSE Workshop & NIS Colloquium EPR in Catalysis: from Model to Real Systems, Torino, 26-27/11/2015. Plenary lecture.
- 262. Pontiroli, D.; Magnani, G.; Gaboardi, M.; Riccò, M.; Pramudita, J.C.; Sharma, N.; Milanese, C. 2nd Parma Nanoday Workshop, Parma (Italy), 03-04/12/2015. Oral presentation.
- 263. Pontiroli, D.; Magnani, G.; Lenti, S.; Gaboardi, M.; Riccò, M.; Milanese, C.; Pramudita, J.C.; Sharma, N. Carbon 2015 conference, Dresda (Germany), 12-17/07/2015. Oral presentation.
- Ridi, F. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Oral presentation.
- Ridi, F.; Fratini, E.; Tonelli, M.; Baglioni, P.; Borsacchi, S.; Martini, F.; Calucci, L.; Geppi, M. 14th International Congress on the Chemistry of Cement, Beijing (China), 13-16/10/2015. Poster.
- Rizzuti, A.; Mastrorilli, P.; Sportelli, M.C.; Cioffi, N.; Picca, R.A.; Agostinelli, E.; Varvaro, G.; Dassisti, M.; Caliandro, R. Amam 2015, International conference on Applied mineralogy and advanced materials, Castellaneta marina (Italy), 07-12/06/2015. Oral communication.
- Russo Krauss, I.; Guida, V.; Gaudino, D.; Grizzuti, N.; Pasquino, R.; D'Errico, G.; Paduano, L. 1st European Conference on Physical and Theoretical Chemistry, Catania (Italy), 14-18/09/2015. Oral presentation.
- 268. Russo Krauss, I.; Haider, S.; Ramaswamy, S.; Parkinson, G. N. 5th International Meeting on Quadruplex Nucleic Acids: G4thering in Bordeaux, Bordeaux (France), 26-28/05/2015. Poster & flash presentation.
- Russo Krauss, I.; Pica, A.; Spiridonova, V.A.; Tateishi-Karimata, H.; Nagatoishi, S.; Sugimoto, N.; Sica, F. 5th International Meeting on Quadruplex Nucleic Acids: G4thering in Bordeaux, Bordeaux (France), 26-28/05/2015. Poster.
- Sacconi, S.; Tadini-Buoninsegni, F.; Moncelli M.R.; Margheri, G.; Cerboneschi, M.; Tegli, S. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
- 271. Salis, A. 5th NanoDrug International Scientific Meeting, Alghero, 28/06/2015-01/07/2015. Invited speaker.
- Salis, A.; Medda, L.; Monduzzi, M. TheoBio 2015, International Theoretical Biophysics Symposium, Cagliari, 08-12/06/2015. Poster.
- 273. Salis, A.; Medda, M.; Monduzzi, M. 29th ECIS Conference, Bordeaux (France), 06-11/09/2015. Poster.
- 274. Santoru, A.; Pistidda, C.; Garroni, S.; Milanese, C.; Marini, A.; Masolo, E.; Bergemann, N.; Le, T.T.; Mulas, G.; Enzo, S.; Klassen, T., Dornheim, M. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications". Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
- 275. Scarano, S.; Carretti, E.; Baglioni, P.; Dei, L.; Minunni, M. XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI) 13-17/09/2015, Trieste. Oral presentation.
- 276. Scarano, S.; Mariani, S.; Ermini, M.L.; Barale, R.; Bonini, M.; Minunni, M. Biophotonics 2015, Florence (Italy), 20-22/05/2015. Oral presentation.
- 277. Singh, M.; Mulla, M.Y.; Manoli, K.; Magliulo, M.; Ditaranto, N.; Cioffi, N.; Palazzo, G.; Torsi, L.; Santacroce, M.V.; Di Franco, C.; Scamarcio, G. 6th IEEE International Workshop on Advances in Sensors and Interfaces, Gallipoli (Italy), 18-19/06/2015. Oral communication.
- Smeazzetto, S.; Young, H.S.; Trieber, C.A.; Moncelli M.R.; Tadini-Buoninsegni, F. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
- Sportelli, M.C.; Ancona, A.; Picca, R.A.; Volpe, A.; Lugarà, P.M.; Cioffi, N. Euroanalysis XVIII, the European Conference on Aalytical Chemistry, Bordeaux 06-10/09/2015. Oral communication.

- Sportelli, M.C.; Ancona, A.; Picca, R.A.; Volpe, A.; Trapani, A.; Trapani, G.; Cioffi, N. Materials Research Society 2015 Spring Meeting, San Francisco, CA (USA), 21-25/04/2015. Oral communication.
- 281. Sportelli, M.C.; Picca, R.A.; Manoli, K.; Magliulo, M.; Re, M.; Pesce, E.; Tapfer, L.; Di Franco, C.; Cioffi, N.; Torsi, L. Materials Research Society 2015 Spring Meeting, San Francisco, CA (USA) 21-25/04/2015. Poster.
- Sportelli, M.C.; Tütüncü, E.; Picca, R.A.; Valentini, M.; Valentini, A.; Kranz, C.; Mizaikoff, B.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Oral communication.
- Strazewski, P.; Fiore, M.; D'Onofrio, A.; Emiliano, A.; Mavelli, F. Syschem 2015, Abdij Rolduc (The Netherlands), 19-22/05/2015. Oral presentation.
- Tadini-Buoninsegni, F.; Moncelli M.R.; Peruzzi, N.; Ninham, B.W.; Dei, L.; Lo Nostro, P. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
- 285. Tadini-Buoninsegni, F.; Moncelli M.R.; Tegli, S. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
- Tamasi, G.; Bonechi, C.; Rossi, C.; Cini, R.; Magnani, A. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
- 287. Tonelli, M.; Martini, F.; Calucci, L.; Fratini, E.; Geppi, M.; Ridi, F.; Borsacchi, S.; Baglioni, P. 15th European Student Colloid Conference, Krakow, 08-11/06/2015. Oral presentation.
- Toulmé, J.J.; Da Rocha, S.; Dausse, E.; Fernandez, P.; Allard, M; Kryza, D.; Janier, M.; Scarano, S.; Crispo, F.; Minunni, M.; Hassan, A.; Paurelle, O.; Azéma, L. OLIGO 2015 Oxford Antisense and therapeutic Nucleic Acids, 30/03/2015, Oxford (UK). Oral presentation.
- Toulmé, J.J.; Dausse, E.; Fernandez, P.; Debordeaux, F.; Kryza, D.; Janier, M.; Scarano, S.; Crispo, F.; Minunni, M. Hassan, A.; Paurelle, O.; Azéma, L. 11th Annual Meeting of the Oigonucleotide Therapeutic Society, 11-14/10/2015, Lieden (The Netherlands). Oral presentation.
- Tovar Rodríguez, J.; Fratini, E. XV Sigma-Aldrich Young Chemists Symposium, SAYCS 2015, Rimini (Italy), 27-29/10/2015. Oral presentation.
- 291. Tovar Rodríguez, J.; Ramírez Hernández, G.Y.; Galindo Esquivel, I.R.; Fratini, E.; De Los Reyes Heredia, J.A. XII European Congress on Catalysis, EUROPACAT 2015, Kazan (Russia), 30/08-04/09/2015. Poster.
- 292. Tuccitto, N.; Zappalà, G.; Vitale, S.; Licciardello, A. International SIMS Conference SIMSXX, Seattle (USA), 2015. Oral presentation.
- Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A; Licciardello, A. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
- Tuccitto, N.; Zappalà, G.; Vitale, S.; Giamblanco, N.; Marletta, G.; Licciardello, A. Secondary Ion Mass Spectrometry SIMS XX, Seattle (USA), 13-18/09/2015. (Poster).
- Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A.; Licciardello, A. Secondary Ion Mass Spectrometry SIMS XX, Seattle (USA), 13-18/09/2015. Poster.
- Valentini, A.; De Pascali, G.; Melisi, D.; Valentini, M.; Cioffi, N.; Casamassima, G. Amam 2015, International conference on Applied mineralogy and advanced materials, Castellaneta marina (Italy), 07-12/06/2015. Plenary lecture.
- 297. Valentini, A.; Fracchiolla, G.; Carbonara, G.; Rosato, A.; Cioffi, N.; Casamassima, G. Amam 2015, International conference on Applied mineralogy and advanced materials, Castellaneta marina (Italy), 07-12/06/2015. Oral communication.
- Venditti, F.; Cuomo, F.; Ceglie, A.; Lopez, F. 15th Conference of the International Association of Colloid and Interface Scientists. Mainz (Germany), 24-29/05/2015. Poster.
- Vitale, S.; Zappalà, G.; Tuccitto, N.; Santoni, M.P.; Campagna, S.; Licciardello, A. Secondary Ion Mass Spectrometry SIMS XX, Seattle (USA), 13-18/09/2015. Oral presentation.
- Zappalà, G.; Vitale, S.; Tuccitto, N.; Licciardello, A. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
- 301. Altamura, E.; Mavelli, F. Syschem 2014, San Sebastian (Spain), 09-12/06/2014. Oral presentation.
- 302. Altamura, E.; Mavelli, F. Working group meeting COST Action CM1304 Compartment Permeability, Parmenides Foundation, Munich (Germany), 20-22/11/2014. Oral presentation.
- 303. Baglioni, P. 1st Soft Matter School, Venice, Isola di S. Servolo, 16-20/06/2014. Invited lecture.
- 304. Baglioni, P. Cultural heritage and advanced technologies Symposium, Italian Institute of Culture,
- London, 13/11/2014. Invited lecture.
- Baglioni, P. Director's Colloquium, University of Canberra, Leonard Huxley Lecture Theatre, Australia, 14/08/2014. Plenary lecture.
- 306. Baglioni, P. Royal Institute of Art, Stoccolma (Svezia), 20-21/03/2014. Invited lecture.
- Baglioni, P. Gordon Conference: Scientific Methods in Cultural Heritage Research, Sunday River Resort in Newry, ME, USA, 27/074-01/08/2014. Invited lecture.
- 308. Baglioni, P. The digital future of world heritage, University of Notre Dame in Rome, 2-4/04/2014.
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Invited lecture

- Baglioni, P. VIII Congresso Nazionale di Archeometria Scienze e Beni Culturali: stato dell'arte e prospettive, CNR, Bologna, 5-7 febbraio 2014. Invited lecture.
- Baglioni, P. Shaanxi Normal University, School of Material Science and Engineering, Xi'an (China), 23-29/08/2014. Invited lectures.
- Baglioni, P. Cracow Academy of Fine Arts in Poland, Faculty of Conservation of Works of Art, Cracow (Poland), 25-28/05/2014. Invited lecture.
- Baglioni, P. ECIS 2014, 28th International Conference of the European Colloid and Interface Society, Limassol (Cyprus), 07-12/09/2014. Invited Keynote.
- 313. Baratto, M.C.; Martorana, A.; Aguila, S.A.; Vazquez-Duhalt, R.; Basosi, R. Oxizymes 2014, Vienna 01-04/07/2014. Poster.
- 314. Basosi, R. Bogazici University Istanbul, 01/04/2014. Plenary lecture.
- 315. Basosi, R. EuCheMS Round Table on Energy, Environment and Food, Rome "La Sapienza", 25/11/2014.
- 316. Basosi, R. London School Of Economics, 03/2014. Plenary lecture.
- 317. Basosi, R. Medaglia D'oro Della SCI, Università della Calabria, 07/09/2014. Invited lecture.
- 318. Basosi, R. Prolusione Apertura 774° A.A. Università di Siena, 16/12/2014. Invited lecture.
- 319. Basosi, R. SET Plan Conference, Roma, 09/12/2014. Plenary lecture.
- 320. Basosi, R. University Of Warsaw, 09/2014. Plenary lecture.
- Bernini, C.; Arezzini, E.; Basosi, R.; Sinicropi, A. XXV Congresso Nazionale della SCI, Arcavacata di Rende (CS), 07-12/09/2014. Poster.
- 322. Bernini, C.; Zani, L.; Calamante, M.; Reginato, G.; Mordini, A.; Taddei, M.; Basosi, R.; Sinicropi, A. XXV Congresso Nazionale della SCI, Arcavacata di Rende (CS), 07-12/09/2014. Poster.
- Berti, D. Balard Chemistry conferences: Self-Assembly of Biomolecules, La Grande Motte (France), 12-15/10/2014. Invited lecture.
- 324. Berti, D. Nanomedicine Symposium CEN@Politecnico: Synthesis of nanomaterials, biological applications and modelling, Politecnico di Milano (Italy), November 2014. Invited lecture.
- 325. Berti, D. Torino (Italia), 10/11/2014. Invited lecture.
- Berti, D. Magnetocubosomes for Controlled Drug Delivery, Politecnico di Milano (Italia), Dicembre 2014. Invited presentation.
- Biancalani, C.; Cerboneschi, M.; Macconi, S.; Moncelli, M.R.; Smeazzetto, S.; Biricolti, S.; Bogani, P.; Tegli, S. XX Convegno Nazionale SIPAV, Pisa (Italy), 22-24/09/2014. Poster.
- 328. Cerboneschi, M.; Lanzini, G.; Macconi, S.; Onor, M.; Campanella, B.; Bramanti, E.; Moncelli, M.R.; Tadini-Buoninsegni, F.; Biricolti, S.; Bogani, P.; Tegli, S. XX Convegno Nazionale SIPAV, Pisa (Italy), 22-24/09/2014. Poster.
- Cioffi, N.; Dilonardo, E.; Di Franco, C.; Afzal, A.; Alvisi, M.; Penza, M.; Palmisano, F.; Torsi, L. COST Action TD1105 - Second International Workshop, ENEA, 25-26/03/2014, Brindisi. Invited Oral communication.
- Cuomo, F.; Lopez, F.; Ceglie, A.; Miguel, M.G.; Lindman, B. 4th International Colloid Conference. Surface Design and Engineering. Madrid (Spain), 15-19/06/2014. Oral presentation.
- Dassisti, M.; Mastrorilli, P.; Rizzuti, A.; Caliandro, R.; Cioffi, N. 1st WORKSHOP on the State of the art and Challenges Of Research Efforts@POLIBA, 03-05/12/2014, Politecnico di Bari (Italy). Poster.
- Del Buffa, S.; Bonini, M.; Ridi, F.; Severi, M.; Losi, P.; Volpi, S.; Al Kayal, T.; Soldani, G.; Baglioni P. EMRS – Fall meeting, Warsaw, 15-19/09/2014. Oral presentation.
- Del Buffa, S.; Rinaldi, E.; Carretti, E.; Bonini, M.; Ridi, F.; Baglioni, P. EMRS Fall meeting, Warsaw, 15-19/09/2014. Poster.
- 334. Dilonardo, E.; Di Franco, C.; Afzal, A.; Ditaranto, N.; Alvisi, M.; Penza, M.; Palmisano, F.; Torsi, L.; Cioffi, N. ISA2014 Incontro di Spettroscopia Analitica University of Bologna, Ravenna (Italy), 05-06/06/2014. Oral communication.
- 335. Dilonardo, E.; Penza, M.; Alvisi, M.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. COST Action TD1105 - New Sensing Technologies for Air-Pollution Control and Environmental Sustainability -Third Scientific Meeting, organized by GEBZE and Bahcesehir University, Istanbul, 03-05/12/2014. Poster.
- 336. Dilonardo, E.; Penza, M.; Alvisi, M.; Di Franco, C.; Suriano, D.; Rossi, R.; Palmisano, F.; Torsi, L.; Cioffi, N. COST Action TD1105 - New Sensing Technologies for Air-Pollution Control and Environmental Sustainability - Third Scientific Meeting, organized by GEBZE and Bahcesehir University, Istanbul, 03-05/2014. Oral communication.
- 337. Dilonardo, E.; Penza, M.; Alvisi, M.; Suriano, D.; Cassano, G.; Palmisano, F.; Torsi, L.; Cioffi, N. EMRS2014 Spring Meeting, Symposium B: Advanced functional materials for environmental monitoring and applications, Lille (France), 26-30/05/2014. Poster.
- Dilonardo, E.; Penza, M.; Alvisi, M.; Suriano, D.; Rossi, R.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. COST Action TD1105 - Second International Workshop, ENEA, 25-26/03/2014, Brindisi. Poster.

- Dilonardo, E.; Penza, M.; Alvisi, M.; Suriano, D.; Rossi, R.; Palmisano, F.; Torsi, L.; Cioffi, N. EMRS2014 Spring Meeting, Symposium B: Advanced functional materials for environmental monitoring and applications, Lille (France), 26-30/05/2014. Oral communication.
- Dilonardo, E.; Penza, M.; Alvisi, M.; Suriano, D.; Rossi, R.; Palmisano, F.; Torsi, L.; Cioffi, N. Secondo Convegno Nazionale Sensori, 19-21/02/2014, Roma (Italy). Oral communication.
- 341. Dilonardo, E.; Penza, M.; Cassano, G.; Alvisi, M.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. XXV Congresso Nazionale della Società Chimica Italiana SCI 2014, Università della Calabria, Arcavacata di Rende (CS), 07-12/09/2014. Oral communication.
- 342. Ditaranto, N.; Picca, R.A.; Sportelli, M.C.; van der Werf, I.D.; Mangone, A.; Cioffi,, N.; Sabbatini, L. ISA2014 Incontro di Spettroscopia Analitica University of Bologna, Ravenna (Italy), 05-06/06/2014. Oral communication.
- 343. Fanti, P.; Giustarini, D.; Rossi, R.; Folli, F.; Khazim, K.; Cornell, J.; Matteucci, E.; Bansal, S. XVII International Congress on Nutrition and Metabolism in Renal Disease, Würzburg (Germany), 06-10/05/2014. Poster.
- Ferrari, S.; Quartarone, E.; Bini, M.; Tomasi, C.; Capsoni, D.; Mustarelli, P. IMLB The 17th International Meeting on Lithium Batteries, Como, 10-14/06/2014. Poster.
- Ferraro, G.; Fratini, E.; Ridi, F.; Baglioni, P. XIV Sigma-Aldrich Young Chemists Symposium, SAYCS 2014, Rimini (Italy), 27-29/10/2014. Poster.
- Garroni, S.; Santoru, A.; Pistidda, C.; Milanese, C.; Masolo, E.; Marini, A.; Dornheim, M.; Mulas, G.; Enzo, S. International Symposium on Metal – Hydrogen Systems MH 2014, Manchester (UK), 20-25/07/2014. Oral presentation.
- Giorgi, R. Conference at CNCPC Coordinación Nacional de Conservación del Patrimonio Cultural; Auditorio de la CNCPC, 21/10/2014. Oral presentation.
- Giorgi, R. Conference at Encrym Escuela Nacional de Restauración, Conservación y Museografía; Sala de Consejos de la ENCRyM, 22/10/2014. Oral presentation.
- 349. Giorgi, R. Conference at Jesuit Church in Lviv (Ukraine), 05/07/2014. Oral presentation.
- 350. Giorgi, R. Conference at UNAM. Instituto de Física, 20/10/2014. Oral presentation.
- 351. Giorgi, R. IMAT conference, Firenze, 12/11/2014. Oral presentation.
- 352. Giorgi, R. Keynote al XXV Congresso Nazionale della Società Chimica Italiana SCI 2014. Arcavacata di Rende Università della Calabria, 07-12/09/2014. Oral presentation.
- Giorgi, R. Keynote alla V Jornada de Conservacao-Restauracao intitolata "Conservacao e Tecnologia: caminhos da Inovacao", Rio De Janeiro (Brasile). 22-24/09/2014. Oral presentation.
- 354. Giorgi, R. La Conservación de la Pintura Mural en Sitios Arqueológicos Problemàtica y Estrategias de Intervención, organizzato da IPCE - School of Conservation of Archeological Wall Paintings. Najera, La Rioja (Spagna), 06-08/05/2014. Oral presentation.
- Giorgi, R. Seminario presso la Universidad Nacional Autonoma de Mexico UNAM. Mexico City, 18/02/2014. Oral presentation.
- Gosalawit-Utke, R.; Meethom, S.; Pistidda, C.; Milanese, C.; Laipple, D.; Saisopha, T.; Marini, A.; Klassen, T.; Dornheim, M. International Symposium on Metal – Hydrogen Systems MH 2014, Manchester (UK), 20-25/07/2014. Oral presentation.
- 357. Grandi, S.; Achilli, C.; Guidetti, G.F.; Ciana, A.; Quartarone, E.; Capsoni, D.; Minetti, G. E-MRS: European Materials Research Society, Lille (France), 26-30/05/2014. Poster.
- Gualdani, R.; Lentini, G.; Moncelli, M.R. 39th FEBS Congress, Paris (France), 30/08/2014-05/09/2014. Poster.
- Gualdani, R.; Tadini-Buoninsegni, F.; Lentini, G.; Moncelli, M.R. XXII Congresso Nazionale SIBPA, Palermo (Italy), 21-24/09/2014. Oral presentation.
- Gualdani, R.; Zanardelli, M.; di Cesare Mannelli, L.; Francesconi, O.; Ghelardini, C.; Nativi, C.; Moncelli, M.R. 39th FEBS Congress, Paris (France), 30/08/2014-05/09/2014. Poster.
- 361. Innocenti, M.; Cinotti, S.; Di Benedetto, F.; Lavacchi, A.; Felici, R.; Carlà, F.; Cioffi, N.; Vizza, F. 65th Annual Meeting of the International Society of Electrochemistry, Symposium 10: Electrodeposition for Energy Applications 31/08-05/09/2014 Lausanne (Switzerland). Invited oral communication.
- 362. Luchini, A.; Vitiello, G.; De Julian Fernandez, C.; Heenan, R.; Montesarchio, D.; D'Errico, G.; Paduano, L. IX Congresso Consorzio internuniversitario dei Sistemi a Grande Interfase (CSGI), Napoli, 01-02/07/2014. Oral presentation.
- 363. Luchini, A.; Vitiello, G.; De Julian Fernandez, C.; Heenan, R.; Montesarchio, D.; D'Errico, G.; Paduano, L. XXV Congresso Nazionale Società Italiana Spettroscopia Neutronica (SISN) – Italian Neutron Scattering Conference, Napoli, 03-04/07/2014. Oral presentation.
- Magliulo, M.; Mallardi, A.; Manoli, K.; Cioffi, N.; Palazzo, G.; Torsi, L. EMRS2014 Spring Meeting, Symposium B: Advanced functional materials for environmental monitoring and applications, Lille (France), 26-30/05/2014. Invited oral communication.
- Maranghi, S.; Parisi, M.L.; Busi, E.; Basosi, R. VIII Convegno della Rete Italiana LCA, Florence, 19-20/06/2014. Poster.



- 366. Mariani, S.; Ermini, M.L.; Scarano, S.; Belissima, F.; Bonini, M.; Minunni, M. COST Thematic workshop Integrated approahces for biomolecular detection: nanostructures, Biosensors and Lab on Chip devices, 28-30/04/2014, Catania (Italy). Poster.
- Mariani, S.; Scarano, S.; Minunni, M. Giornata scientifica di Bioanalitica, Chimica Bioanalitica per La Sicurezza Ambientale ed Alimentare, Bologna, 04/07/2014. Poster.
- Mariani, S.; Scarano, S.; Spadavecchia, J.; Minunni, M. Xxv Congresso Della Societa' Chimica Italiana, Rende 08-12/09/2014. Oral presentation.
- Marletta, G.; Messina, G.M.L.; Giamblanco, N. N.I.C.E. 2014, 2nd International Conference on Bioinspired and Biobased Chemistry and Materials, Nice (France), 15-17/10/2014. Oral presentation.
- Martina, M.R.; Menichetti, S.; Procacci, P.; Caminati, G. International Conference Nanotech Italy 2014, Venice, 26-28/11/2014. Oral presentation.
- Mavelli, F. 2nd International Summit on Integrative Biology, Chicago (USA), 04-05/08/2014. Invited oral presentation.
- 372. Mavelli, F. IX Congresso Annuale del Consorzio Interuniversitario per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), Napoli, 01-02/07/2014. Oral presentation.
- 373. Mavelli, F.; Altamura, E. Syschem 2014, San Sebastian (Spain), 09-12/06/2014. Oral presentation.
- Mavelli, F.; Altamura, E. Working group meeting COST Action CM1304 Compartment Permeability, Parmenides Foundation, Munich (Germany), 20-22/11/2014. Oral presentation.
- Mavelli, F.; Altamura, E.; Stano P. CoSMoS Satellite Workshop of ALIFE 14, New York (USA), 29-30/07/2014. Oral presentation.
- Messina, G.M.L.; Karakeçili, A.; Marletta, G. GRC Biointerface Science 2014, Lucca (Italy), 16-20/06/2014. Poster.
- Messina, G.M.L.; Karakeçili, A.; Marletta, G. MRS Fall Meeting & Exhibit, Boston (USA), 29/11/-06/12/2014. Poster.
- Meucci, V.; Minunni, M.; Vanni, M.; Sgorbini, M.; Intorre, L. Atti SISVet LXVIII. vol. LXVIII, p. 24-25, Pisa, 16-18/06/2014. Poster.
- Milanese, C.; Aramini, M.; Gaboardi, M.; Pontiroli, D.; Girella, A.; Marzaroli, V.; Riccò, M.; Marini,
 A. International Symposium on Metal Hydrogen Systems MH 2014, Manchester (UK), 20-25/07/2014. Poster.
- Milanese, C.; Girella, A.; Marini, A.; Aramini, M.; Gaboardi, M. Pontiroli, D.; Riccò, M. CIMTEC 6th Forum on New Materials, Montecatini Terme (Italy), 08-13/06/2014. Oral presentation.
- Minunni, M. Seconda Scuola Nazionale sui Biosensori Ottici e Biofotonica, Otranto (Italy) 15-20/09/2014. Oral presentation.
- Monduzzi, M.; Medda, L.; Salis, A. 28th ECIS Conference, Limassol (Cyprus), 07-12/09/2014 Oral presentation.
- Murgia, S.; Caltagirone, C.; Falchi, A.M.; Meli, V.; Monduzzi, M.; Prodi, L.; Schmidt, J.; Talmon, Y. 28th ECIS Conference, Limassol (Cipro), 07-12/09/2014. Oral presentation.
- Parisi, M.L.; Spinelli, D.; Pogni, R.; Basosi, R. VIII Congresso Nazionale dell'AIGE Associazione Italiana Gestione Energia, Reggio Emilia (Italy), 09-10/06/2014. Oral presentation.
- Picca, R.A.; Calvano, C.D.; Sportelli, M.C.; Fazio, B.; Priolo, F.; Irrera, A.; Cioffi, N. MRS2014 Spring Meeting, San Francisco, CA (USA), 21-25/04/2014. Poster.
- Picca, R.A.; Sportelli, M.C.; Dilonardo, E.; Cioffi, N. IX Congresso del Consorzio per lo Sviluppo dei Sistemi a Grande Interfase – CSGI, Napoli (Italy), 01-02/07/2014. Oral communication.
- 387. Pogni, R. Nanoday, Siena, 25/06/2014. Oral presentation.
- 388. Pogni, R. Oxizymes 2014, Vienna, 01-04/07/2014. Oral presentation.
- 389. Pogni, R. XIX Scuola Nazionale di Chimica bioinorganica per dottorandi, Pisa, 22-24/10/2014. Plenary lecture.
- 390. Pogni, R.; Baratto, M.C.; Sinicropi, A.; Ruiz-Dueñas F.J.; Sáez-Jiménez, V.; Linde, D.; Martínez, A.T.; Basosi, R. XXV Congresso Nazionale della SCI, Arcavacata di Rende (Italy), 07-12/09/2014. Poster.
- 391. Pontiroli, D.; Gaboardi, M.; Magnani, G.; Aramini, M.; Milanese, C.; Pramudita, J.C.; Sharma, N.; Riccò, M. 2nd International Congress on Energy Efficiency and Energy Related Materials (ENEFM), Oludeniz (Turkey), 16-19/10/2014. Oral presentation.
- Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M.; Bertoni, G.; Milanese, C. 1st Parma Nanoday Workshop, Parma (Italy), 28/11/2014. Oral presentation.
- 393. Quinzeni, I.; Ferrari, S.; Quartarone, E.; Capsoni, D.; Mustarelli, P.; Bini, M. E-MRS: European Materials Research Society, Lille (France), 26-30/05/2014. Poster.
- Ridi, F. Riunione Scientifica Annuale delle Unità Operative del Consorzio CSGI, Napoli, 01-02/07/2014. Oral presentation.
- Rizzuti, A.; Mastrorilli, P.; Dassisti, M.; Sportelli, M.C.; Picca, R.A.; Cioffi, N. XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Università della Calabria, Arcavacata di Rende (CS), 07-12/09/2014. Poster.
- 396. Russo Krauss, I.; Parkinson, G.; Merlino, A.; Randazzo, A.; Novellino, E.; Mattia, C.A.; Mazzarella,

L.; Sica, F. Functional DNA Nanotechnology Workshop, Rome (Italy), 19-20/06/2014. Poster & flash presentation.

- 397. Russo Krauss, I.; Pica, A.; Merlino, A.; Mazzarella, L.; Sica, F. Functional DNA Nanotechnology Workshop, Rome (Italy), 19-20/06/2014. Poster & flash presentation.
- Russo Krauss, I.; Pica, A.; Merlino, A.; Sica, F. XXV Congresso Annuale della Società Italiana di Spettroscopia Neutronica (SISN), Napoli (Italy), 03-04/07/2014. Poster.
- Salis, A.; Medda, L.; Casula, M.F.; Monduzzi, M. Realizing Reformulation a Symposium on Surface and Materials Chemistry, Lund, 22-24/10/2014. Poster.
- 400. Salis, A.; Medda, L.; Cugia, F.; Parsons, D.F.; Ninham, B.W.; Monduzzi, M. 28th ECIS Conference, Limassol (Cyprus), 07-12/09/2014. Oral presentation.
- Salis, A.; Medda, L.; Monduzzi, M. SiO2, Advanced Dielectrics and Related Devices, Cagliari, 15-18/06/2014. Oral presentation.
- 402. Santoru, A.; Garroni, S.; Pistidda, C.; Milanese, C.; Masolo, E.; Marini, A.; Dornehim, M.; Mulas, G.; Enzo, S. International Symposium on Metal – Hydrogen Systems MH 2014, Manchester (UK), 20-25/07/2014. Poster.
- Scarano, S; Mariani, S.; Minunni, M. XXV Congresso della Società Chimica Italiana, Rende, 08-12/09/2014. Poster.
- 404. Scarano, S.; Mariani S.; Minunni, M. 1st IMEKO FOOD Promoting Objective and measurable Food Quality and Safety – Rome (Italy), 13-15/10/2014. Oral presentation.
- 405. Scarano, S.; Mariani, S.; Minunni, M. International conference on Biophysics, section Bioispired nanotechnologies and Biosensors, RBC 2014 in Smolenice castle, 15-20/05/2014. Oral presentation.
- 406. Smeazzetto, S.; Cerboneschi, M.; Thiel, G.; Moncelli, M.R. Course on Biophysics of Channels and Transporters, Erice (Italy), 11-17/05/2014. Poster.
- Smeazzetto, S.; Moncelli, M.R.; Thiel, G. 58th Biophysical Meeting, San Francisco (USA), 15-19/02/2014. Poster.
- Sportelli, M.C.; Hoetger, D.; Picca, R.A.; Manoli, K.; Kranz, C.; Mizaikoff, B.; Torsi, L.; Cioffi, N. EMRS2014 Spring Meeting, Symposium B: Advanced functional materials for environmental monitoring and applications, Lille (France), 26-30/05/2014. Poster.
- 409. Sportelli, M.C.; Hötger, D.; Picca, R.A.; Manoli, K.; Kranz, Mizaikoff, B.; Torsi, L.; Cioffi, N. MRS2014 Spring Meeting, San Francisco, CA (USA), 21-25/04/2014. Oral communication.
- 410. Sportelli, M.C.; Nitti, M.A.; Valentini, M.; Picca, R.A.; Melisi, D.; Bonerba, E.; Sabbatini, L.; Tantillo, G.; Valentini, A.; Cioffi, N. XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Università della Calabria, Arcavacata di Rende (Italy), 07-12/09/2014. Oral communication.
- 411. Sportelli, M.C.; Picca, R.A.; Manoli, K.; Magliulo, M.; Torsi, L.; Cioffi, N. XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Università della Calabria, Arcavacata di Rende (Italy), 07-12/09/2014. Keynote.
- Sportelli, M.C.; Picca, R.A.; Manoli, K.; Torsi, L.; Cioffi, N. Società Chimica Italiana & SIGMA ALDRICH Young Chemists Symposium, 14th edition Riccione (Italy), 27-29/10/2014. Oral communication.
- Stefan, A. Convegno: Valorizzazione dei co-prodotti come scelta strategica per la sostenibilità delle bioraffinerie da colture dedicate, Ecomondo, Rimini (Italy), 07/11/2014. Oral presentation.
- Stefan, A.; Boiani, M.; Longanesi, L.; Hochkoeppler, A. 16th European Congress on Biotechnology, Edinburgh (UK), 13-16/07/2014. Poster.
- 415. Stefan, A.; Montòn-Silva, A.; Ceccarelli, A.; Hochkoeppler, A. Conference, Zing Conferences, Cambridge (UK), 31/08-04/09/2014. Poster.
- 416. Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R.; Inesi, G.; Sitsel, O.; Gourdon, P.; Meloni, G.; Nissen, P. 14th International Conference 'Na,K-ATPase and related transport ATPases: Structure, mechanism, cell biology, health and disease', Lunteren (The Netherlands), 30/08-05/09/2014. Oral presentation.
- 417. Vitale, S.; Zappalà, G.; Leanza, D.; Napolitani, E.; Licciardello, A. SIMS Europe 2014 IX European Workshop on Secondary Ion Mass Spectrometry, Muenster (Germania), 07-09/09/2014. Poster.
- 418. Vitiello, G.; D'Errico, G.; Silipo, A.; Molinaro, A.; Paduano, L. IX Congresso Consorzio internuniversitario dei Sistemi a Grande Interfase (CSGI), Napoli (Italy), 01-02/07/2014. Oral presentation.
- Vitiello, G.; Luchini, A.; Heenan, R.K.; Silipo, A.; Molinaro, A.; D'Errico, G.; Paduano, L. XXV Congresso Nazionale Società Italiana Spettroscopia Neutronica (SISN) – Italian Neutron Scattering Conference, Napoli (Italy), 03-04/07/2014. Oral presentation.
- Vitiello, G.; Luciani, G.; Costantini, A.; Silvestri, B.; Avossa, J.; D'Errico, G.; Pezzella, A.; Paduano, L.; Branda, F. IX Conferenza Consorzio internuniversitario dei Sistemi a Grande Interfase (CSGI), Napoli (Italy), 01-02/07/2014. Poster.
- 421. Zappalà, G.; Motta, V.; Vitale, S.; Torrisi, A.; Licciardello, A. SIMS Europe 2014 IX European Workshop on Secondary Ion Mass Spectrometry, Muenster (Germania), 07-09/09/2014. Oral presentation.



Attività Editoriale

- Amedeo Marini Editorial Board member of Journal of Pharmaceutical Sciences (Wiley).
- Andrea Salis Associate Editor of *Biocatalysis* (De Gruyter).
- Claudia Crestini Editor of the *Journal of Applied Chemistry* (Hindawi); Guest editor of *Bioresources* (NC State University); Advisory Board member of *Cellulose Chemistry and Technology Journal* (EAR).
- Claudiu T. Supuran Editor-in-Chief of the following: Expert Opinion on Therapeutic Patents
 (Taylor & Francis), Journal of Enzyme Inhibition and Medicinal Chemistry (Taylor & Francis),
 Current Enzyme Inhibition (Bentham Science), Antiinflammatory and Antiallergy Agents in
 Medicinal Chemistry (Bentham Science); Senior Editor of Infectous Diseases-Current Topics in
 Medicinal Chemistry (Bentham Science); Editorial Board member of the following: ACS Med
 Chem Lett (ACS), European Journal of Medicinal Chemistry (Elsevier), Bioorganic and
 Medicinal Chemistry (Elsevier), Bioorganic and Medicinal Chemistry (Elsevier), Current
 Medicinal Chemistry (Bentham Science), Molecules (MDPI), Current Pharmaceutical Design
 (Bentham Science), Current Organic Chemistry (Bentham Science), Metal Based Drugs
 (NCBI), International Journal of Molecular Science (John Wiley & Sons), Turkish Journal of
 Biochemistry (De Gruyter), Marine Drugs (MDPI), Journal of Molecular Recognition (Wiley),
 Applied Organometallic Chemistry (Wiley), Anticancer Agents in Medicinal Chemistry
 (Bentham Science), Metabolites (MDPI).
- Debora Berti Ownership Board member of *Physical Chemistry Chemical Physics* (Royal Society of Chemistry); co-Editor in Chief of *Journal of Colloid and Interface Science* (Elsevier).
- Giovanni Marletta Advisory Board member of the *Journal of Applied Biomaterials & Functional Materials* (Wichtig).
- Luigi Paduano Associated Editor of Journal of Solution Chemistry (Springer).
- Luisa Torsi Regional Editor for Europe di Flexible and Printed Electronics (IOP).
- Maria Minunni Editorial Board member of *Sensing and Bio-Sensing Research* (Elsevier); Review Editor of *Frontiers in Chemistry*.
- Nicola Cioffi Editorial Board member of the following: Research & Reviews in ElectroChemistry (Trade Science Inc.), The Open Materials Science Journal (Bentham Science), Sensor Letters (ASP), Journal of Sensors (Hindawi); co-Guest Editor of Molecules (MDPI) e Nanomaterials (MDPI).
- Piero Baglioni Editorial Board member of *European Physical Journal E* (Springer); Associate Editor of *Physical Chemistry Chemical Physics* (Royal Society of Chemistry); Advisory Board member of the following: *Journal of Colloid Interface Science* (Elsevier), *Langmuir* (ACS).
- Roberto Piazza Senior Editor of Journal of Physics Condensed Matter per Liquids, Soft Matter, Biological Physics (Iop Science).
- Sergio Murgia Editorial Board member of BioMed Research International (Hindawi).

Organized/Chaired

- The Research Unit of CSGI-Catania, on behalf of the EuChemS division of Physical Chemistry and Physical Chemistry Division of the Società Chimica Italiana, has organized the 1st European Conference on Physical, Theoretical, and Computational Chemistry and XLII Annual Meeting of the Physical Chemistry Division of SCI, Catania (Italy), September 14-18, 2015. The Conference hosted more than 170 attendees from 15 countries, featuring 12 international Invited Speakers, more than 70 Oral presentations and 112 Poster presentations.
- Structure and Dynamics of Supercooled Water and Other Glassy Materials, Palermo, 09-11/10/2015.

Guests

- Yosef Scolnik (IYAR-Israel Institute for Advanced Research), 29/11/2016: "Deviation from identity of macroscopic properties of enantiomers via water chiral preference. Is water chiral?".
- Maria Vallet-Regì (Departamento de Quimica Inorganica y Bioinorganica, Universidad Complutense de Madrid), 10/11/2016: "Biomaterials Design"; 16/11/2016: "Smart Nanosystems".
- Gavin Walker, Energy Technologies Research Institute, University of Nottingham. "Multicomponent Hydride Systems for Hydrogen Storage Applications". 15/11/2016.

- Mohammed Harir, Ph.D. Student (fellowship from the Ministery of Higher Education of Algeria), 01/10/2015–09/10/2016 "Molecular characterization of extracts produced by strains of Actinobacteria isolated from Algerian Sahara soil".
- Flor Guadalupe Sánchez Alejandro, Ph.D student (Doctorante del Programa en Ciencias de la Vida Biotecnología Marina) from CICESE/CNyN, UNAM, Mexico, 1/05/2016-31/07/2016 "EPR spectra on three derivatives of versatile peroxidase with aromatic aminoacids in order to characterize the radical intermediates formed".
- Pierre Joseph (Centre national de la recherche scientifique CNRS, Laboratory for Analysis and Architecture of Systems – LAAS), 01/09/2015-31/07/2016.
- Barbara Lonetti (Centre national de la recherche scientifique CNRS, Laboratoire des Interactions Moléculaires et Réactivité Chimique et Photochimique – IMRCP-UMR 5623), 01/09/2015-31/07/2016.
- Ignacio Rene Galindo Esquivel (Departamento de Ingegnería Química, Universidad de Guanajuato), 19/09/2015-20/07/2016.
- Stephen T. Hyde (Department of Applied Mathematics, Australian National University), 05/07/2016: "Animal, Vegetable, Mineral. A continuum of form".
- Marco Casazza, Siena 31/05/2016 "Atmospheric aerosol pollution an old concern, some new perspectives". Seminario.
- Elsa Callini, Laboratory of Materials for Renewable Energy, EPFL, Switzerland. "Stabilization of gas species via incorporation in porous solids". 29/01/2016.
- Miriam Rueda Noriega, High Pressure Processes Group Dept. Chemical Engineering and Environmental Technology University of Valladolid. "Enhanced hydrogen storage material by stabilization of a hydride in microparticles of silica aerogel". 10/12/2015.
- Huiping Xing (School of Material Science and Engineer, Shaanxi Normal University, China), 01/09/2014-30/09/2015.
- Kondo Francois Aguey-Zinsou, Materials Energy Research Laboratory in Nanoscale School of Chemical Engineering The University of New South Wales Sydney, Australia. "From size effects to functional hydrogen stores". 14/09/2015.
- Curtis W. Frank (Stanford University, Department of Chemical Engineering), 01/01/2015-31/07/2015.
- Jolanta Polak, Researcher (Marie Curie-Skłodowska, University Lublin, Poland) 25-30/05/2015 "Novel phenazines with antimicrobial properties synthesized by fungal laccase from Cerrena unicolor".
- Ángel Martín, High Pressure Processes Group Dept. Chemical Engineering and Environmental Technology University of Valladolid. "Development of new materials using compressed fluids". 26/11/2014.
- Rodolfo Guillermo Valle Altamirano, Master student (Instituto de Biotecnologia, Universidad Nacional Autonoma de Mexico, Medicina Molecular y Bioprocesos, Cuernavaca), 17/05/2014–15/06/2014
 "Spectroscopic Analysis of the H2O2- resistant Zo Peroxidase Alternative Ground State (GS*) and Compound III (CIII) Species".
- Etsuo Akiba, Department of Mechanical Engineering, Faculty of Engineering, Kyushu University, Nishi-ku, Fukuoka, Japan. "Hydrogen storage and transport: State-of-art in Japan". 13/06/2014.
- Marzia Pentimalli, Laboratorio di Chimica e Tecnologie dei Materiali, ENEA, Centro Ricerche Casaccia, Roma, "Sviluppo di un sistema di refrigerazione a idruri metallici alimentato da calore di scarto. Caratterizzazione termodinamica dei materiali e definizione del ciclo termico". 15/05/2014.
- Kostas Hatzixanthis (Director of Research Procarta Biosystems Ltd, Norwich, UK), 21/01/2014: "Development of nanoparticulate Nucleic-Acid based Therapeutics, Snares[™], for the treatment of infectious diseases and an introduction to EU IAPP project DNA-TRAP".

Theses (undergraduate, master and PhD)

U.O. Bari

Bachelor in Chemistry (Laurea triennale)

- Lapenna, A.: "Sviluppo di un metodo di immobilizzazione di glicoenzimi in idrogel di alginato per applicazioni ensoristiche" (2014).
- Angelini, G.: "Immobilizzazione dell'enzima Tirosinasi da Agaricus Bisporus mediante deposizione via plasma a pressione atmosferica di un film polietilenico" (2016).
- del Sole, R.: "Controlled deposition of gold nanoparticles for Laser Induced Breakdown Spectroscopy applications" (2016).

Bachelor in Materials Science (Laurea triennale)

• Talamo, S.: "Studio preliminare della immobilizzazione di enzimi mediante deposizione via plasma a pressione atmosferica di coating polimerici" (2016).

Master in Chemistry (Laurea magistrale)

• Dilucca, M.: "Studio microstrutturale di un sistema tensioattivo commercial" (2016).

Master in Materials Science and Technology (Laurea magistrale)

- Angarano, V.: "Studio sull'immobilizzazione di enzimi mediante deposizione di coating polimerico via plasma a pressione atmosferica" (2016).
- Cimmarusti, G.M.: "Cellulose gelation in confinement" (2016).

PhD in Chemical and Molecular Sciences

• Sportelli, M.C.: "Synthesis and advanced morphological-spectroscopic characterization of transition metal nanostructures and their application in analytical methods" (2016).

U.O. Bologna

Bachelor in Industrial Chemistry (Laurea triennale)

- Perrone, A.: "Sovraespressione in Escherichia coli del sub-assemblaggio $\tau \alpha \epsilon \theta$ della DNA polimerasi III" (2014).
- Perticarari, S.: "Caratteristiche biochimiche e fenotipiche della variante D201A del dominio PHP della subunità α di Escherichia coli" (2014).
- Camerani, M.: "Sovraespressione e parziale purificazione di una DNA polimerasi di Deinococcus radiodurans" (2015).
- Caramia, S.: "Caratterizzazione cinetica di β-glucosidasi di Prunus dulcis" (2015).
- Maturi, M.: "Purificazione e caratterizzazione della DNA Polimerasi α di Deinococcus radiodurans" (2015).
- Del Grosso, I.: "Sovraespressione e purificazione della subunità α della DNA polimerasi III di Escherichia coli" (2016).

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• Ottone, P.: "Tecniche analitiche in campo enologico" (2016).

Master in Industrial Chemistry or Molecular and Industrial Biotechnologies (Laurea magistrale)

- Lapenta, F.: "Caratterizzazione dell'attività pirofosfatasica associata al dominio PHP della DNA polimerasi III" (2014).
- Magri, L.: "Espressione eterologa e purificazione della istone deacetilasi umana 1 (HDAC1)" (2014).
- Martina, C.E.: "Dal frammento Klenow a HoLaMa. Ingegnerizzazione di una mini DNA polimerasi di Escherichia coli" (2014).
- Rossi, N.: "Sintesi di PNA a libertà conformazionale ridotta" (2014).
- Schipani, F.: "Sovraespressione in Escherichia coli e purificazione della istone deacetilasi umana 1 (HDAC1)" (2014).
- Tetter, S.: "Supercharged ferritin as a nanotechnological tool and transfection agent" (2014).
- Fontana, M.: "Characterization of nanofluidics devices for high-throughput single molecule fluorescence detection" (2015).
- Rocca, M.: "In vitro engineering and assembly of an artificial carboxysome" (2015).
- Perrone, A.: "Sovraespressione, purificazione e caratterizzazione cinetica della polimerasi DnaE di Deinococcus radiodurans" (2016).
- Perrucci, J.: "Sovraespressione di sub-assemblaggi della DNA polimerasi III di Escherichia coli mediante la co-trasformazione dell'ospite con plasmidi compatibili" (2016).

PhD in Biotechnological and Pharmaceutical Sciences

• Montòn Silva, A.: "Structural and kinetic characterization of DNA polymerases I and III from Escherichia coli" (2015).

U.O. Cagliari

Bachelor in Chemistry (Laurea triennale)

- Fanti, S.: "Silice mesoporosa ordinata funzionalizzata con biopolimeri come possibile sistema drug delivery. Importanza del grado di funzionalizzazione sulle proprietà strutturali e tessiturali" (2015).
- Pruner, S.: "Adsorbimento di biomolecole su Materiali Mesoporosi Ordinati" (2015).

Master in Chemical Sciences (Laurea magistrale o a ciclo unico)

- Carucci, C.: "Hofmeister phenomena in Bioelectrochemistry: The supporting Electrolyte Affects the Response of Glucose Electrodes" (2014).
- Tocco, F.: "Materiali Mesoporosi Ordinati per l'Immobilizzazione di Antibiotici" (2014).
- Becconi, O.: "Studio delle interazioni specifiche tra Li+, Na+, K+ e l'albumina del siero bovino mediante dinamica molecolare" (2016).
- Collu, M.: "Fenomeni Hofmeister in biocatalisi. Effetti specifici degli anioni sulla sintesi enzimatica del biodiesel" (2016).



- Delpiano, G.R.: "Sintesi e caratterizzazione di sistemi multifunzionali costituiti da nanoparticelle di silice mesoporosa coniugate con proteine e nanoparticelle d'oro" (2016).
- Magnolia, S.: "Sistemi "stimuli-responsive" per il drug delivery: effetto del pH su nanoparticelle di silice mesoporosa funzionalizzate con acido ialuronico" (2016).
- Medda, S.: "Studio dell'interazione tra l'albumina di siero bovino e nanoparticelle di silice mesoporosa funzionalizzate con biopolimeri" (2016).
- Sedda, S.: "Effetto degli elettroliti sull'adsorbimento fisico del lisozima su materiali a base di silice mesoporosa" (2016).

PhD in Chemical Sciences and Technologies

 Meli, V.: "Theranostic applications of fuorescent liquid crystalline nanoparticles" (2016).

U.O. Campobasso

Bachelor in Agriculture, Environment, Food (Laurea triennale)

- Tata, S.: "Ecogenicità e rilascio da liposomi indotto dal pH" (2015).
- Meli, V.: "Messa a punto e caratterizzazione di microsfere di proteine di soia-zeina per il trasporto nutraceutico controllato" (2016).

Master in Agriculture, Environment, Food (Laurea magistrale)

• Tucci, R.: "Interventi di mitigazione del rischio di liquefazione su larga scala" (2016).

U.O. Catania

Bachelor in Chemistry (Laurea triennale)

- Leanza. D.: "Ancoraggio di sistemi fotoattivi su substrati di TiO2 nanostrutturati" (2014).
- Livio, P.: "Preparazione e caratterizzazione morfologica ed elettrica su scala nanometrica di 'nastri' macromolecolari di Poli-3-esil-tiofene (P3HT)" (2015).
- Lo Bello, L.: "Ancoraggio di molecole fotoattive su substrati flessibili" (2015).
- Moschetto, S.: "Preparazione e caratterizzazione di film sottili ibridi di nanotubi di carbonio e polimeri coniugati" (2015).
- Valenti, A.M.G.: "Ancoraggio di sistemi fotoattivi su substrati nanostrutturati di SnO2" (2015).
- Fichera, L.: "Metodologie di "patterning" di monolayer fosfolipidici " (2016).
- Lombardo, T.: "Sintesi stepwise, su superfici di ossidi, di sistemi organici per elettronica molecolare" (2016).
- Ruffino, R.: "Metodologie di riconoscimento selettivo di monosaccaridi in matrici biologiche modello" (2016).

Master in Materials Chemistry (Laurea magistrale)

• Eredia, M.: "Caratterizzazione chimica spazialmente risolta di sistemi organici micro- e nano- strutturati mediante ToF-SIMS" (2014).

- Scollo, M.: "Preparazione e studio di film sottili di miscele di semiconduttori organici per applicazioni fotovoltaiche" (2014).
- Tummino, A.: "Nano/Meso strutturazione e caratterizzazione di superfici polimeriche" (2014).
- Condorelli J.: "Assemblaggio e caratterizzazione di film ultrasottili per l'elettronica molecolare" (2015).
- Russo, M.R.: "Preparazione e caratterizzazione di materiali per packaging innovativo in microelettronica" Tesi in collaborazione con ST Microelectronics (Catania) (2015).
- Spampinato N.: "Caratterizzazione chimica tridimensionale di sistemi ibridi microstrutturati mediante cluster-SIMS" (2015).
- Barillaro, S.: "Materiali elettrodici per Batterie Redox a Flusso di Vanadio" Tesi in collaborazione con ITAE/CNR (Messina) (2016).

PhD in Materials Science

• Zappalà, G.: "Assembly and characterisation of molecular films for energetics and electronics" (2014).

U.O. Firenze

Bachelor in Chemistry (Laurea triennale)

- Gelli, R.: "Mineralizzazione di idrogel macroporosi a base di imogolite e gelatina" (2014).
- Grifoni, E.: "Nanocompositi biodegradabili a base di polisaccaridi e nanoargille: preparazione, caratterizzazione e studio delle proprietà di rilascio" (2014).
- Pastacaldi, G.: "Sintesi di nanoparticelle di silice mesoporose per il consolidamento di opere d'arte" (2014).
- Rinaldi, E.: "Nanocompositi iniettabili a base di Halloysiti e Polisaccaridi" (2014).
- Santini, S.: "Studio degli effetti di pH e specie fosfato su idrogel di PAAm" (2014).
- Sordi, G.: "Studio dell'interazione di un composto del platino con Ca-ATPasi" (2014).
- Magnani, C.: "Comprensione delle proprietà antibatteriche di agenti terapeutici nanostrutturati tramite interazione con modelli di membrane Gram-negative" (2015).
- Tanteri, V.: "Preparazione e caratterizzazione di nanocompositi biodegradabili a base di poliidrossibutirrati, polossameri e Halloysiti" (2015).
- Bolognesi, A.: "Studio degli effetti dell'addizione di alloisiti funzionalizzate su cementi a base di magnesio" (2016).
- Brandi, F.: "Caratterizzazione chimico fisica di un fluido nanostrutturato per la rimozione di film polimerici" (2016).
- Cialli, O.: "Fluidi nanostrutturati per il dewetting di film polimerici da superfici di interesse per i beni culturali" (2016).
- Giannetti, C.: "Studio dell'interazione di esametafosfato con cementi a base di silicati idrati di magnesio" (2016).
- Nardin, R.: "Gel filmogeni a base di PVA per la rimozione di patine da reperti in bronzo" (2016).



- Perdichizzi, A.: "Studio delle interazioni di cementi a base di magnesio con fasi alluminatiche" (2016).
- Salvi, M.: "Nanocarriers a Base di Complessi di Ioni Rame" (2016).

Bachelor in Diagnostics and Materials for Conservation and Restoration (Laurea triennale)

- Alterini, M.: "Rimozione selettiva di ridipinture in Arte contemporanea mediante gel chimici" (2015).
- Donatelli, A.: "Reperti archeologici copti: caratterizzazione dei materiali impiegati nel restauro" (2015).
- Guerini, L.: "Deacidificazione non acquosa di manoscritti contenenti inchiostri sintetici" (2015).
- Onorato, F.: "Dispersioni non acquose di lattato di calcio per la stabilizzazione del pH di manufatti a base di collagene" (2015).
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U.O. Napoli

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U.O. Siena

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Theses

RESEARCH PROJECTS

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1A – Spontaneous aggregation of soil organic matter and its interaction with iron oxide particles

R. Angelico, G. Palumbo, C. Colombo, J. He (Centre for Ecoenvironmental Sciences, Chinese Academy of Sciences, Beijing, China)

Aims

Chemical and physicochemical behaviour manifested by humic acid (HA) in natural soil and water environments is a function of its molecular structure, and dictates its organic matter mobility, interaction with clay surfaces, and aggregation in natural environments. In the present research project, Atomic Force Microscopy in contact mode (AFM-C) was used to investigate the aggregate conformation of leonardite humic acid (HA) formed at different pH values in the range 2-12. Computational molecular models of HA, based on its chemical composition as determined by NMR measurements, were also analyzed to provide a possible conformation of 3D supramolecular structure and were compared to AFM results.

Finally, we extended our investigation to the HA coprecipitation process with iron (II) oxide and studied its effect on the iron (hydr)oxide crystallinity.

Results

The structure of HA aggregates adsorbed on mica observed in AFM micrographs showed a considerable dependence on the pH of the solutions used in the preparation of the colloidal dispersions. Interestingly, HA solubilized at pH 5 showed a ring shaped supramolecular structure. (a) AFM-C 2D microtopography, (b) and c) 3D microtopography images of HA dispersed in water at pH 5 adsorbed and air-dried on a mica surface. (d) Heights of individual HA particles observed with AFM-C plotted vs. their measured lengths.



Based on molecular simulation methods, the molecular conformation of HA was performed on the Lignin–Carbohydrate Complex (LCC) model in which the parameters of the β -O-4 linkages in the oligomeric chain were optimized. The LCC model provided a possible conformation of the 3D ring structure of HA, depending on the pH employed in its preparation. These results were very helpful to understand the influence of carboxylic and phenolic group ionization on the HA molecular arrangement in terms of size, strength, and flexibility. Covalent and hydrogen bonds appeared to stabilize the oligomeric chain of the helical structure, while dipole–dipole and van der Waals interactions held the ring-like conformation. The proposed model was a significant step toward a full understanding of HA structure and function.



Molecular modelling results: (a) Overlapping helical structures formed by three subunits of the phenyl propanoid chain linked in a regular linear sequence, (b) Linear structure formed from two overlapped chains composed of six units, (c) 45–50 linear helix molecules looped spirally to form a ring-shaped structure. Finally, an experimental investigation performed through Transmission electron Microscopy (TEM), X-ray Diffraction (DRX) and Diffuse Reflectance Spectroscopy (DRS) was carried out to analyse the microstructure of synthetic iron coprecipitates in solid state and while their colloidal behavior as a function of pH was ascertained through Photon Correlation Spectroscopy and Laser Doppler electrophoresis.

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1A – Adhesion promoters for bitumen

R. Angelico, C. Oliviero Rossi, B. Teltayev (Kazakhstan Highway Research Institute, Almaty, Kazakhstan)

Aims

All asphalt pavements consist of two main components, bitumen and mineral aggregate. The function of bitumen, which typically represents 4-7 wt % of the pavement, is to act as a binder in-between the aggregate skeleton, giving the asphalt sufficient internal cohesion. It is, therefore, of vital importance that the bitumen has a strong bond (adhesion) to the aggregate surface. In the present project, we investigate the interactions at the bitumen-aggregate interface when different types of adhesion promoters are premixed to the bitumen.

Results

From research in the road construction sector, the most common types of activators present on the market are classified according to the chemical nature of their active ingredient: amides, PolyPhosphoric Acid (PPA) esters and organosilanes. Therefore, for each of these families, the adhesive properties of the corresponding modified bitumen loaded with a fixed amount of active agent, were tested on four types of stone materials. X-Ray Powder Diffractometry (XRPD), X-Ray Fluorescence (XRF) and Environmental Scanning Electron Microscope Energy Dispersive Spectroscopy (ESEM-EDS) were carried out in order to establish the chemical and mineralogical nature and identify the agglomerate structures of the selected inert rocks. Among various screened products, the organosilane-based additive showed excellent adhesive performances, independently of the chemical composition of inorganic interfaces, as confirmed by both contact angle and boil test measurements (Figure 1).



Fig. 1: Contact angles of bitumen without additives and mixed with additives, measured for various investigated aggregate surfaces: I: Quartz monzogabbro; II: White marble; III: Metamorphite; IV: Limestone.

As expected, the performance of the adhesion promoters based on amide and ester of the PPA was strongly influenced by the chemical nature of the stones. This behaviour is consistent with the formation of specific chemical interactions in the adhesion process between bitumen and aggregate. On the other hand, one can argue that the

bituminous mixture based on the organosilane additive interacts with aggregates through a different mechanism driven by physical rather than chemical interactions, as confirmed by the absence of any dependence of contact angle on the type of inert stone. Therefore, the addition of 0.1 wt % organosilane to bitumen enhances remarkably its wettability onto the inert rock, independently of its chemical compositions and surface charge characteristics (either acid or basic types). Conventional boiling test results confirmed the highest coating rate recorded for the organosilane-modified bitumen, whereas samples formulated with amide and PPA ester adhesive promoters provided lower degrees of coating, as they were affected by the chemical nature of inert stones.



Pristine bitumen



Bitumen + 0.1 wt % PPA ester



Bitumen + 0.1 wt % organosilane



Bitumen + 0.1 wt % amide

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1A – Design, synthesis and applications of new organic sensitizers for non-conventional photovoltaic cells

A. Sinicropi, M.L. Parisi, S. Maranghi, R. Basosi

Aims

The aim of the project is the design, computational characterization and synthesis of new organic dyes for the production of Dye Sensitized Solar Cells, along with the environmental assessment of their photovoltaic performances trough life cycle analysis.

Results

Since the pioneering work published by Grätzel and O'Reagan on the first efficiently assembled dye-sensitized solar cell (DSSC) in 1991, the research activity on photovoltaic cells based on hybrid sensitizer/nanocrystalline semiconductor systems has undergone some major developments. This present project is based on a multidisciplinary approach for the production of new organic dye sensitizers for DSSCs that could result to be competitive in comparison with the already available solar systems. This approach takes benefit from the synergic employment of state-of-the-art computational methods and innovative eco-compatible synthetic strategies that together with the spectro-, photo- and electrochemical characterization of the synthesized compounds allows the development of an accurate protocol for the design and investigation of organic sensitizers to be employed in photovoltaic cells.



A life cycle analysis of the production process of each components of a solar cell has to be performed in order to achieve a systematic and in-depth assessment of environmental impacts and burdens (in energetic and pollution terms) deriving from all input flows, and to highlight the critical points and hot spots of the process itself. Such an evaluation represents the starting point to draw a detailed eco-profile of innovative technologies and their potential applications. Major outcomes from the project are pivotal in understanding the environmental dynamics, the benefits and

drawbacks associated with the production and employment of DSSCs in comparison with other photovoltaic crystalline silicon and other thin film technologies.



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1A – Production and characterization of photoactive materials

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Aims

Production of a fiber with sufficient and long-lasting photoactivity and mechanical properties.

Results

Sources for indoor air pollution are cleaners, waxes, paints, pesticides, adhesives, cosmetic products, automotive products, and hobby supplies. Conventional methods to remove pollution are often ineffective, chemically and energetically intensive and suitable only for large systems. An alternative is represented by photocatalysis. TiO2, ZnO_1 , ZrO_2 , CdS_1 , MoS_2 , Fe_2O_3 , and WO_3 have been used as photocatalyst and among them, titanium dioxide remained the benchmark against which alternative photocatalysts are compared. However, TiO2 nanoparticles have recently been classified by the International Agency for Research on Cancer (IARC) as an IARC Group 2B carcinogen "possibly carcinogenic to humans.". Therefore, the identification of polymeric photoactive compounds is recommended in order to reduce health problems induced by nanoparticle handling. Photocatalysts prevent the deterioration of textiles caused by insects, fungi, algae, and microorganisms. The selfcleaning property of a photoactive textile is based on the discoloration of organic stains by reactive radicals. Photocatalytic oxidation (PCO) is an emerging technology in air purification, and is also based on the decomposition of harmful substances. The use of photocatalytic textiles in antimicrobial, self-cleaning, and anti-pollution products are based on the highly reactive radicals that are generated under band-gap light irradiation.

In this study, SPEEK/PP-based photoactive fibers are manufactured to provide antimicrobial, self-cleaning, and anti-pollution properties. The fibers are made in a melt spinning process, first on laboratory scale and then on a semi-industrial scale.

SEM micrograph of PP (A), SPEEK (B), SPEEK/PP 2:98 (C), SPEEK/PP 5:95 (D), and SPEEK/PP 10:90 (E)



Melt spun SPEEK/PP 5:95 filaments



The fibers are characterized regarding their mechanical properties, photochemical effectiveness, and morphology.

Based on the obtained results, their suitability in commercial textile applications is estimated. In addition to the new polymer-based textile material, the novelty of this study is the melt spinning of an unconventional polymer blend containing two totally different components and time-dependent processability. Chemical modifications of PEEK, such as sulfonation, enhance its solubility in organic solvents through electrophilic substitution reactions and promote the formation of benzophenone ketyl radicals (BPK) that could be effectively used to promote photocatalytic reactions. In fact, UV irradiation of a polar benzophenone induces an n to p* transition generating a triplet state that is highly reactive toward hydrogen atom abstraction by forming a stable radical. A hydrogen transfer reaction is involved in the initial production of the appropriate hydrogen transfer agent depends on the kinetics of H-atom transfer agent and on the stabilisation of the radical induced by the chemical groups on the acceptor. Polyolefins possess a labile hydrogen atom and can therefore act as efficient chain transfer agents, whilst the sulfonated group stabilizes the radicals.



In order to evaluate the photocatalytic effectiveness of the made polymer blends, EPR spectroscopy was performed. Room temperature EPR analysis performed on a transparent casted film made from 100% SPEEK showed that after exposure to UV irradiation for 15 min free radicals are generated. The presence of PP in the SPEEK sample with increasing molar ratio significantly improves the radical formation efficiency. Stable BPK radical was detected and the characterization of the stability of the radical over several irradiation cycles was carried out. The next goal is therefore to estimate the antimicrobial, antipollution, and self-cleaning performance of the final fabrics in order to fully characterize the efficiency of the new fibers.

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1A – Ordered Mesoporous Silica in Nanomedicine: Effect of Functionalization and Interactions with Proteins

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Aims

Synthesis, characterization and functionalization of ordered mesoporous silica. Adsorption and in vitro release of model drugs and proteins. Visualization of adsorbed proteins.

Results

Ordered mesoporous silica (OMS) materials are receiving great attention for nanomedicine applications. OMS can be used to prepare smart depot systems for several kinds of therapeutic agents as, for example, therapeutic proteins. We focused on two types of OMS: SBA-15 and MCM-41. The former is constituted by microparticles with a pore size of about 6-7 nm. The latter is constituted by nanoparticles with a pore size of 2-3 nm. We first studied the interactions between functionalized SBA-15 mesoporous silica and lysozyme, an antimicrobial protein. In order to improve the bioadhesion properties of SBA-15 particles, they were functionalized with hyaluronic acid. SBA-15 samples having high (H-SBA) and low (L-SBA) levels of functionalization were analyzed during the three steps of the preparations: 1. introduction of the $-NH_2$ groups to obtain the SBA-NH₂ samples; 2. functionalization with hyaluronic acid to obtain the SBA-HA matrices; 3. adsorption



of lysozyme. The whole of the experimental data suggests that a high level of functionalization of the silica surface allows for a negligible lysozyme adsorption mainly due to unfavorable electrostatic interactions (H-SBA-NH₂) or steric hindrance (H-SBA-HA). A low degree of functionalization of the silica surface brings about a very good

performance towards lysozyme adsorption, being 71 % (L-SBA-NH₂) and 63 % (L-SBA-HA) respectively, compared to that observed for original SBA-15. A key issue is to prove that a therapeutic protein is effectively able to penetrate the pores of OMS during the adsorption step. To this purpose we immobilized an antibody fragment [F(ab')GAMIgG] conjugated with ultrasmall gold nanoparticles (GNPs) onto amino-functionalized SBA-15 (SBA-NH₂) mesoporous silica. In order to visualize the location of the conjugates adsorbed onto SBA-NH₂ with transmission electron microscopy (TEM), due to the ultrasmall size of GNPs <1 nm, we used a silver enhancement procedure to amplify their size. In this procedure, ultrathin sections of conjugate-loaded SBA-NH₂ particles are firstly prepared. The ultrasmall GNPs located on the top side of the 70–90 nm thick slices act as microcrystallization nucleation sites for the deposition of reduced metallic silver. Consequently, the ultrasmall GNPs increase their size. This allows for the direct imaging of the

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conjugates adsorbed. We clearly localized the F(ab')GAMIgG–GNPs conjugates inside the mesopores of SBA–NH₂ through TEM.

Then we focused on mesoporous silica nanoparticles (MSNs), based on the MCM-41 mesoporous matrix. They were functionalized with amino groups,



and then with hyaluronic acid (HA) or chitosan (CHIT) to fabricate bioactive conjugates. The role of the functional groups towards cytotoxicity and cellular uptake was investigated using 3T3 mouse fibroblast cells. A very high biocompatibility of MSN-NH₂, MSN-HA and MSN-CHIT was assessed through the MTS biological assay and Coulter counter evaluation. No significant differences in cytotoxicity data aroused from the presence of different functional groups in the investigated MSNs. Significant differences due to type of functionalization were instead observed both in the fluorescence microscopy experiments performed with the FITC-conjugated MSN-NH₂, MSN-HA and MSN-CHIT, and in the transmission electron microscopy experiments performed on slices of the investigated systems embedded in epoxy resins. MSN-NH₂, MSN-HA conjugates were easily internalized, being the uptake of the -HA functionalized much higher than that of the -NH₂ functionalized MSNs, whereas MSN-CHIT conjugates gave large aggregates dispersed in the medium or localized at the external surface of the cell membranes. Both fluorescence microscopy and TEM images gave clear evidence that the MSNs are distributed in the cytoplasm of the cells in the case of MSN-NH₂ and MSN-HA, whereas only few particles are internalized in the case of MSN-CHIT.



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1A – Carbon based nanostructures for innovative hydrogen storage systems

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Aims

Ideation and preparation of novel Carbon-based nanostructures and composites for solid-state H_2 storage; evaluation of their sorption properties; determination of the thermodynamic and kinetics characteristics of the sorption reactions.

Results

Thanks to this project (funded by Fondazione Cariplo; number of the grant 2013-0592), started in April 2014 and ended in September 2016, we were able to demonstrate to the scientific community that alkali-cluster intercalated fullerides really constitute a novel class of materials for hydrogen storage, thanks to their proved capability to uptake reversibly high amounts of hydrogen via a complex chemisorption mechanism. We optimized the synthesis of Li, Na, and mixed Li-Na clusters intercalated fullerides, belonging to the families Na_xLi_{12-x}C₆₀ ($0 \le x \le 12$; we were the first group to explore these stoichiometries) and Na_xLi_{6-x}C₆₀ ($0 \le x \le 6$) by solid state methods, obtaining high purity and good reversibility.

The structural properties of the materials were clarified by means of in-situ neutron diffraction and the analysis of the Pair Distribution Function (PDF) obtained from high-energy synchrotron diffraction. The mechanism of hydrogenation was unveiled by Muon Spin Relaxation spectroscopy (µSR), a very powerful technique "able to see hydrogen" in the structures. Thanks to these two methods, we were able for the first time to explain the chemisorptions mechanism leading to the hydrogenation of fullerene in these structure: Li atoms help the dissociation of the hydrogen molecules on the C structures, acting as catalyst and destabilizing agent, but then capture some hydrogen in the formation of LiH. Na atoms act as a more powerful catalyst and does not hydrogenate by itself, but is not able to decrease the working temperature of the C structure. Thanks to our work, we demonstrate the importance to prepare mixed stoichiometries richer in the Li side to obtain good kinetic and thermodynamic properties. By coupled manometric - calorimetric analyses and thermogravimetric measurements, we proved that in these composites C60 covalently binds up to 5 wt% H₂ at moderate temperature and pressure, reaching properties similar to those of Mg hydride, the first generation material for hydrogen storage.

We also identified some strategies to further improve the absorption performance in this class of materials. For example, we succeeded to catalyze Li-fullerides with Pt and Pd nanoparticles, whose known activity towards hydrogen dissociation allows to increase the H_2 absorption up to 5.9 wt% H_2 and of about 35 % the absorption rate with respect to the pure undoped compounds.

Finally, we demonstrated that the Li decorated compounds have also very good properties for ammonia storage, a very hot topic concerning new fuels and energy vectors transportation and use.

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1A – Reversible hydrogen sorption for borohydrides infiltrated in silica matrices

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Aims

To realize borohydrides nanoconfinement in silica based matrices as a way to improve the reversibility and the kinetics of the H_2 sorption reactions of these complex hydrides materials; to optimize the nanoconfinement procedures; to prepare doped matrices and doped compounds to be infiltrated to further improve the hydrogen sorption kinetics.

Results

Borohydrides are very promising materials for solid state hydrogen storage thanks to their high hydrogen content (the theoretical gravimetric capacity is higher than 10 wt%, with the Department of Energy ultimate target for the whole storage tank being 6 wt %). Unfortunately, these materials suffer of poor reversibility and ciclability and work at very high temperature and hydrogen pressure (600 °C, 100 bar).

One promising way to obtain mild sorption conditions and improve the kinetics of the sorption reactions is to encapsulate the hydrogen storage systems in high porous matrices able to confine the active powders in their channels and pores, so forcing them to react in nanometric form with hydrogen gas. Few is still known on the hydrogen sorption mechanism of the powders in these conditions and the encapsulation methods are to be developed and optimized for each single borohydride, due to the different chemico-physical and solubility properties of each of them.

Concerning the borohydrides choice, we decided to start the investigation with the Mg compound $Mg(BH_4)_2$, since it is a very high-capacity hydrogen complex hydride $(14.84 \text{ wt\% of } H_2)$ but its H_2 sorption reversibility remains a challenge. Its thermodynamics of dehydrogenation is calculated to be near ideal for effective hydrogen storage, but experiments reveal competing decomposition pathways with the formation of very stable intermediates limiting the lifecycle. In practice, 11 wt% H₂ reversibility was demonstrated at very high pressures and temperatures, while only 2.5wt% H₂ is exchanged at reasonable conditions. Concerning the matrices, after having demonstrate that C based materials like graphene and nanotubes react with this compound, we decided to try with silica aerogels. The group in Madrid is able to prepare these particles tuning the surface area and the pores size. Due to the properties of Mg borohydride, that melts and decomposes contextually, we cannot use the traditional melt infiltration technique. For this reason, we developed an original solid state high pressure procedure able to force the hydride to go in the silica channels in its hydrogenated form without melting and decomposition, by working at 300 °C and 110 bar of hydrogen (the borohydride melts at T higher than 350 °C at 1 bar of hydrogen pressure). The ex-situ BET, XRPD and IR spectroscopy help to understand the success and extent of encapsulation. Calorimetric measurements are used to describe the thermodynamic features of the

system. The hydrogen sorption performance is explored by cycling the samples in the manometric apparatus under vacuum/up to 110 bar for des/absorption at the characteristic temperatures.

In the 1:1 molar ratio borohydride:silica encapsulated system, a decrease in the dehydrogenation temperature by 60 °C with respect to the pure hydride and a single decomposition step in the range of 220-400 °C is observed. The kinetics of dehydrogenation at 300 °C in the first cycle is two times faster compared to that of the bulk borohydride. 50 % of reversibility for the hydrogen sorption reaction is shown from the first to the second cycle and maintained in the 3rd one: this is the first time a so high reversibility degree is observed in Mg borohydride systems in the relatively mild working conditions proposed in our work.

We are now trying to develop a wet chemistry method for encapsulate the borohydride in the silica matrix by using a suitable solvent able to dissolve both the components without decomposition and easy to remove after the infiltration. THF gave good results concerning the encapsulation yield but demonstrated to be very hard to remove, decreasing the gravimetric capacity of the system.

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1A – Nanostructured scaffolds for tissue engineering

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Aims

Driving cell adhesion, spreading and proliferation by controlled nanometric biofunctionalization at solid surfaces and nanostructured hydrogels.

Recent Results

We have developed novel bioactive titanium implants, based on the anchoring of a layer of ionic-complementary self-assembling peptides (EAbuK) on Ti surfaces, which have been previously sandblasted and acid-etched. The peptide layer is anchored to the metal by covalent functionalization of titania with the self-assembling sequences (see Scheme 1).



Scheme 1: Sequence of the steps for the preparation of the different surfaces.

The peptide layer may also host a substantial amount of the Insulin-like Growth Factor-1, which can efficiently incorporated within the peptide layer. To the construct can also be added a conjugate biomimetic system obtained by chemo-selective ligation between EAbuK and a sequence of 25 residues containing 4 GRGDSP motifs per chain. XPS studies confirmed a change in the surface composition in agreement with the proposed decorations, while contact angle measurements showed a substantial change in wettability induced by the anchored peptide layer. Accordingly, the human osteoblast adhesion and proliferation assays showed an increase in adhesion for the surfaces enriched with conjugate at a concentration of $3.8 \ 10^{-7}$ M and

an enhanced proliferation for samples enriched with Insulin-like Growth Factor-1 at the highest concentration tested (2.1 $10^{-5}M$). Further studies on the role of the different aggregation forms of various classes of ionic-complementary self-assembling peptides (EAbuK) are being investigated, both experimentally, looking at their nanoscale structure as a function of the nature of surfaces, environmental pH and electrical charges at surfaces, and in silico, by means of a mixture of Quantum Mechanical methods and Molecular Dynamic simulation.

In a parallel way, a series of methods have been developed to functionalize at nanoscale bioceramic surfaces, in order to boost efficient processes of biomineralization.



Fig. 2: Functionalisation scheme: silanisation and covalently binding of ALP on alumina substrates with N-hydroxysuccinimide (NHS) and 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC). b) Enzymatic activity of ALP immobilised in alumina discs (ASNEA) measured by pNPP assay immediately after immobilisation at three different temperatures (4 °C, 25 °C and 37 °C). Unfunctionalised alumina discs (A) were used as reference.

Thus, a bioinspired approach to induce self-mineralisation of bone-like material on alumina surfaces has been developed in collaboration with researchers of Brema University. The mineralising enzyme alkaline phosphatase (ALP) was covalently immobilised by a carbodiimide-mediated chemoligation method. The enzymatic activity of immobilised ALP and its mineralisation capability were investigated at acellular conditions as well as in the presence of human bone cells. Analytical, biochemical, immunohistochemical characterization show that ALP is efficiently immobilized, retains its activity and can trigger calcium phosphate mineralization on alumina at acellular conditions. In vitro cell tests demonstrate that ALP functionalized alumina clearly boosts and enhances bone cell mineralization (see fig.2). Our results underpin the high potential of ALP-functionalized alumina for the development of bioactive surfaces for applications such as orthopedic and dental implants, enabling potentially a fast and firm implant Osseo integration.

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1A – Nanohybrids P3HT-based systems

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Aims

Conjugated polymeric composites with carbon nanotubes, in view of the high aspect ratio volume/surface, are expected to behave as optimal conducting materials at relatively low carbon contents. Many applications can be forecast for conjugated polymer/carbon nanotubes hybrid materials, including energy storage and energy conversion devices, sensors, etc.

Recent results

Poly(3-hexylthiophene)/carbon nanotubes composites (P3HT/NTs) are in the forefront of the research on electroactive polymers, due to their recognized role as active elements in organic photovoltaic and OFET/OLED devices. Among this class of materials, the hybrid systems based on single-walled carbon nanotubes (P3HT/SWNTs) deserve a particular interest with respect to the framework of molecular electronics, in view of the expected optimal electronic conductivity and efficiency. We have prepared high conductivity nanohybrid networks of poly(3-hexylthiophene) and single-walled carbon nanotube (P3HT/SWNTs) by spin coating deposition.





Fig.1: P3HT-SWNTs nanohybrids network deposited at 2000 RPM on IDEs.

Fig. 2: I-V characteristics of nanohybrids networks deposited on IDEs at increasing spin-coating speeds (legend reports the respective RPM).

2D networks prepared at high spinning speed showed a conductivity three orders of magnitude higher than that measured for networks deposited at low spinning speed, although the individual nanotubes are not seen to form a direct connection between the electrodes.

The strong improvement of the conductivity performances is accounted for in terms of the formation of a new nanohybrid system, consisting in thin sheaths of P3HT wrapped around SWNTs, forming complex SWNT/P3HT/SWNT junctions yielding a soldering effect of the interposed P3HT sheath.



Fig. 3: The nanometric P3HT wrapping layer, therefore, acts as a conductive glue at the nanotube-nanotube junctions, allow easy tunneling of charge carriers across them.

The results open the way to molecular electronics devices exploiting the long-range conduction capability of nanotubes together with the thin P3HT sheath short range soldering effect at the hybrid nanowire junctions.

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1A – Calcium phosphate-based nanostructures: synthesis in composite materials, stabilization and interaction with biologically relevant Soft Matter

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Aims

Calcium phosphate (CaP) is one of the most important biomaterials, given its essential role played in human body structure and functioning. Learning from Nature, Soft Matter can be successfully used to guide the formation of nanostructured CaPs, and the understanding of the interactions taking place between these minerals and Soft Matter itself is of special interest both in chemistry and nanomedicine. This project aims at preparing and characterizing biomimetic and nanostructured calcium-based phosphates, in order to investigate the interactions that take place between these nanostructures and biologically relevant macromolecules belonging to Soft Matter family.

Results

Inorganic nanostructured phosphates, especially calcium and magnesium-based, are essential components of the human body, since they contribute to maintain its structure and guarantee the proper functioning. CaP is the main inorganic component of human hard tissues and can be found in nanocrystalline form in bone and teeth, embedded in a soft proteic matrix. In amorphous form, CaP is present in casein micelles in human breast milk and its deposition is also involved in several pathological calcifications, such as renal calculi and atherosclerotic plaques. Mg and phosphate-based minerals are biologically relevant too, given their presence in salivary gland stones and kidneys calculi. Moreover, it has been recently found that nanoparticles of endogenous amorphous calcium phosphate formed from coprecipitation with magnesium in intestine (CaMgP) act as chaperones in the transport of macromolecules, such as orally fed protein antigens and bacterial peptidoglycan, to immune cells of intestinal tissue. The relevance of CaP nanostructures in human body, that emerges from the above mentioned examples, makes it a material of paramount importance; its applications in nanomedicine include tissue engineering, materials for dental and orthopedic applications, drug delivery and DNA transfection. Beyond its numerous applications, the study of the formation and characterization of CaPs nanostructures is important per se, to improve our understanding of the biomineralization process and to investigate the interactions that take place between these nanostructures and biologically relevant macromolecules.

In this framework, we investigated the formation of CaP-based nanostructures in different biocompatible polymeric matrices, taking advantage of biomimetic approaches and investigating their templating action in the crystallization of CaP and in presence of inorganic fillers. We studied the formation of hydroxyapatite nanocrystals on a macroporous gelatin hydrogel crosslinked with a bis-epoxide reactant (glycerol diglycidyl ether) and embedded with inorganic clay nanotubes-imogolites. These nanotubes have a two-fold action, acting both as inorganic fillers of the polymeric matrix and as nucleation sites for the growth of hydroxyapatite

nanocrystals. We found that the presence of imogolite promotes the formation of CaP and affects the type of crystalline phase formed.



The formation of CaP was also investigated in crosslinked Gelatin/PVA hydrogels, examining the mineral phase formed by soaking the hydrogel in a simulated body fluid, *i.e.* a solution with ionic concentration close to human plasma. In addition to polymers, this project aims at investigating how biologically relevant macromolecules belonging to Soft Matter affect and tune the precipitation of CaP and if and how they stabilize a specific crystalline phase: for this purpose, we take into account proteins, such as casein, and polysaccharides.

A significant part of this research is also devoted to the stabilization of the amorphous CaP phase: co-precipitation of CaP with Mg²⁺ ions allows the formation of amorphous CaMgP nanoparticles that mimic the biogenic nanostructures that are produced in our gut. The investigation of the interactions between these nanoparticles and complex systems, such as bacteria, can give insights about their puzzling role in our organism.

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1A – Advanced nanostructured materials for eco-sustainable cements: investigation of the structural properties and innovative strategies for their improvement

M. Tonelli, E. Fratini, F. Ridi, P. Baglioni

Aims

Structural characterization of MgO/SiO_2 cements. Simultaneous hydration of traditional Portland cement and eco-sustainable MgO-based cements. Multi-technique investigation on the kinetic of the process and the hydration products.

Results

We studied mixtures prepared by simultaneous hydration of Portland cement (C) and MgO/SiO₂ (MS) in different weight proportion, providing a physico-chemical characterization of the complex processes that occur and a detailed structural characterization of the formed amorphous binder phases. These formulations are promising in view of two compelling environmental issues: reducing the large CO₂ emissions associated to Portland production and the encapsulation of nuclear waste. The combination of TG/DTA, XRD, FT-IR and SEM analyses elucidated the effects of composition on the formation of the silicate binder phases magnesium and calcium silicate hydrate (M-S-H and C-S-H), which, in agreement with previous works, resulted to be substantially phase separated, as evident from the SEM images on the right.

The hydration kinetic of the samples was followed over one month by reporting the free water index (FWI) as a function of time. A combination of the Boundary Nucleation and Growth Model (BNGM) with the three-dimensional diffusional model was used to describe the curves, as shown in the figure below.

Results demonstrate that the hydration of the magnesium- and of the calcium-based components affect each other: low amounts Portland cement in MgO/SiO₂ mixtures accelerate and enhance M-S-H precipitation, while low amounts of MgO/SiO₂ in Portland cement mixtures accelerate and enhance C-S-H precipitation. It could be possible to control the formation of calcium and magnesium silicate hydrate gels and the pH of the final material, which is



fundamental in order to predict its behaviour in geological repositories for radioactive waste disposal, by mixing proper amounts of MgO/SiO_2 and Portland powders. We further performed a comprehensive structural characterization of MgO/SiO_2



cements using а multi-technique approach, including a detailed solid-state NMR investigation and, in particular, for the first time, quantitative ²⁹Si solid-state NMR data (performed in the framework of the collaboration with F. Martini, L. Calucci, S. Borsacchi and M. Geppi from the University of Pisa and ICCOM CNR of Pisa). Upon mixing highly reactive MgO and SiO₂ with water at room temperature, the binder gel phase M-S-H precipitates within the first 24 hours of hydration, and its amount increases over

the entire monitored period of 1 month. The reaction proceeds through the hydration of MgO to give $Mg(OH)_2$, which then reacts with silica. Analysis of the data reveals that this reaction results in the formation of an amorphous phase that is constituted by an intimate mixture of subnanometer-sized "chrysotile-like" (*left figure*) and "talc-like" (*right figure*) sub-nanometric domains, which are approximately in a 1:1 molar ratio after long-time hydration (in the figure blue tetrahedra represent Si species; red, yellow and white spheres represent O, Mg and H atoms, respectively). This assessment of the M–S–H structure paves the way for tailoring the macroscopic properties of eco-sustainable cements by means of a bottom-up approach.



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1A – A green integrated microwave-assisted synthesis of hexagonally ordered silica sieves using a geothermal waste as silicon source

J. Tovar Rodriguez, E. Fratini, P. Baglioni

Aims

Development of an innovative eco-friendly synthesis of mesoporous silicates using a silicon waste as silicon source. Microwave irradiation (MW) for thermal activation and hydrothermal synthesis. Design of green integrated synthesis approach.

Results

A sample of inorganic geothermal waste was used as Silicon precursor for the preparation of mesoporous silicates. The green synthesis of the materials was performed by hydrothermal treatment, using a microwave-assisted Teflon-lined stainless steel high-pressure reactor. MW irradiation was applied in-situ by means of an innovative microwave coaxial antenna, which allows direct microwave application within the reaction system¹. The following figures show the Small Angle X-Ray Scattering patterns for all prepared sieves under conventional (*left*) and MW (*right*) heating:



For comparative purposes, hexagonal MCM-41 was also prepared using tetraethoxysilane as conventional silicon source. Calcined MCM-41 features four main scattering peaks in the scattering vector interval from 0.05 to 0.5Å⁻¹, that can be assigned to the diffraction peaks of the (100), (110), (200) and (210) planes, associated to the hexagonal structure *p6mm* group². The as-received geothermal waste features no ordering in the explored q vector range whereas the prepared mesoporous sieves exhibit a main scattering peak centered at around the same q vector value for MCM-41. Other two less resolved scattering peaks are observed and can be interpreted as the convolution of the (110) and (200) peaks, and the Bragg reflection of the (210) plane respectively. The intensity of the latter seems to increase as the total hydrothermal treatment time increases. Interestingly, after only two hours of MW hydrothermal synthesis it is possible to yield a material with a fair degree of ordering. Another interesting feature is the formation of surface silanol groups in the material.

The ²⁹Si NMR spectra are shown on the left diagram for the starting raw material and the hexagonal silicate. The geothermal waste has a sole spectral signal with a maximum at -112ppm (using TMS as standard) indicative of Q⁴ siloxane species. For the mesoporous sieve, two other signals are observed at around -102 and -92 ppm associated to the resonances of Q³ and Q² nuclei, corresponding to isolated and geminal silanol groups (Si(OH) and Si(OH)₂ surface groups). Considered as weak catalytic Bronsted sites, the reactivity of the silanol moiety is particularly important for surface functionalization or grafting of these silicates.



The textural properties for all prepared materials were evaluated by means of Nitrogen adsorption and desorption isotherms. Table 1 summarizes the lattice cell parameters, BET surface area and pore volume for all calcined solids. The geothermal waste by itself has a low surface area of 45m²/g. MCM-41 prepared under conventional heating conditions achieves a BET area of 655m²/g after 24h of hydrothermal treatment while MW prepared samples exhibit areas ranging from 500 up to 700m²/g as the total HT time increases from 2h to 6h. For comparative

purposes, MCM-41 prepared using the alkoxide shows a BET area of $923m^2/g$. Pore volume also increases with the hydrothermal treatment time, ranging from 0.55 to 0.70cm³/g for microwave prepared materials. The d₁₀₀ and a₀ lattice cell parameters were estimated using the main Bragg diffraction peak from the SAXS curve and its value depends on the surfactant used as structure directing agent, the degree of hydrolysis of the silicon source that was used and the hydrothermal treatment time.

Table 1. Textural properties and lattice cell parameters for the prepared mesoporous sieves

Sample	HT time, h	BET Area, m ² /g	Pore vol. ml/g	d ₁₀₀ , Å	a ₀ , Å
GeoWaste	0	45	0.22	0	0
GeoMCM_MW2h	2	504	0.55	38.7	44.6
GeoMCM_MW4h	4	546	0.69	43.3	50.1
GeoMCM_MW6h	6	707	0.70	43.7	50.5
GeoMCM_ConvHT24h	24	655	0.62	45.5	52.5
MCM-41_TEOS	24	923	0.80	44.8	51.7

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1A – Microwave assisted synthesis of hexagonally ordered mesoporous silica modified by isomorphic incorporation of Yttrium

J. Tovar Rodriguez, E. Fratini, P. Baglioni

Aims

Modification of MCM-41 by isomorphic incorporation of Yttrium in the hexagonal framework. Characterisation of the textural properties of the mesoporous sieves.

Results

Yttrium-modified hexagonally ordered mesoporous silica sieves were prepared under hydrothermal conditions in a microwave-assisted synthesis approach. Hexadecyl trimethyl ammonium bromide was used as structure directing agent and tetraethoxysilane as silicon source. A series of synthesis gels were prepared with the following molar ratios: $Si(OC_2H_5)$: $xYN_3O_9*6H_2O$: 0.30 CTABr : 185 H_2O : 21.5 NH₃, Where x is the Y/Si nominal molar ratio for the desired final material and it was selected as 0.02, 0.04, 0.06 and 0.08, in order to preserve the hexagonal ordering of the pure siliceous MCM-41 parent material. Figure 1 shows the FTIR spectra (*left*) and the Small Angle X-Ray Scattering curves (*right*) for all prepared materials:



Fig. 1: FTIR spectra (left) and SAXS curves (right for Yttrium modified mesoporous silicates).

Unmodified MCM-41 features a main transmission band centered at around 1048cm⁻¹ that can be associated to the internal Si-O-Si stretching vibrations¹ of the silicon tetrahedrons within the hexagonal structure. As a consequence of Yttrium incorporation, the possible formation of Si-O-Y bond may result in a band intensity reduction and its shift to a wavenumber value of 1070cm⁻¹, suggesting a successful Yttrium substitution. No significant changes are observed for the intensity of the bands located at around and 973 and 796cm⁻¹ which are associated to the asymmetrical (v_{as} (Si-O-Si)) and symmetrical (v_{symm} (Si-O-Si)) stretching modes.

Concerning the structural features, bare MCM-41 exhibits four well-resolved scattering peaks centered around the q vector values of 0.16, 0.28, 0.32 and 0.43 Å⁻¹, which can be assigned to the Bragg diffraction peaks for the (100), (110), (200) and (210) planes associated to the hexagonal structure², *p6mm* group. As the amount of

Yttrium increases, the degree of hexagonal ordering of the material decreases. Considering the covalent atomic radii (1.11 Å for Si and 1.90 Å for Y)³ the lower degree of hexagonal ordering of the materials may be explained by an effective isomorphic substitution of larger Y atoms in the hexagonal framework. Since TEOS addition is given in a dropwise step, Y^{3+} species may interact with the partially hydrolyzed silane forming Si-O-Y covalent bonds before polymerizing around the micellar arrangements of the template. Table 1 summarizes the lattice cell parameters and textural properties for all xY-MCM-41 materials.

Table 1. Lattice cell parameters and textural properties of calcined x-Y-MCM-41 materials						
Sample name	d ₁₀₀	a ₀	$S_{BET} Area,$	Total pore	Monolayer	Pore
	(nm)	(nm)	m²/g	volume ml/g	volume, ml/g	Diameter, nm
MCM41	4.46	5.15	1181	1.05	271	3.54
0.02YMCM41	4.47	5.16	693	0.77	159	4.44
0.04YMCM41	4.59	5.30	757	0.90	174	4.78
0.06YMCM41	4.78	5.52	663	1.06	152	6.39
0.08YMCM41	5.08	5.87	563	0.81	130	5.74

The textural properties were evaluated by means of nitrogen physisorption. An example of a typical isotherm is show on diagram a). All samples exhibit a type IV isotherm according to the IUPAC classification. As the amount of substituted Yttrium increases in the silica network, the pore enlarges up to 60% to a final value of 5.74nm in size. surface area The total in consequence, decreases with the pore broadening. The parent material MCM-41 features a BET area of 1180m²/g and its value decreases swiftly to $563m^2/g$ for 0.08-Y-MCM-41.



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1A – Tuning the pore size, surface area and hydrophobicity of template-based mesoporous silica SBA-15

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Aims

Tuning the pore size, pore volume and surface area of mesoporous hexagonally ordered silica SBA-15. Surface grafting for enhanced hydrophobicity.

Results

Mesoporous silica SBA-15 was synthesized by hydrothermal treatment using a nonionic surfactant Pluronic P123 ($EO_{20}PO_{70}EO_{20}$) as structure directing agent and tetraethoxysilane as silicon source. In order to tailor the dimensions of the pore size, 1,3,5-trymethylbenzene (TMB) was used as swelling agent with the following TMB/P123 w/w ratios: 0.08, 0.16, 0.33 and 1.0. After the formation of the synthesis gel, the hydrothermal synthesis was carried out in the temperature interval from 80° to 120°C and autogenous pressure. Textural properties were obtained by nitrogen adsorption/desorption isotherms and are shown below:

Table 1. Lattice cell parameters and textural properties for large pore silicas

Material	TMB/P123	BET Surface	Pore size [‡] ,	d ₁₀₀ ,	a ₀ , nm	Pore Volume,
	w/w ratio	Area, m ² /gr	nm	nm		ml/g
SBA-15	0	781	4.76	10.3	11.89	0.82
SBA-15-80 [§]	1	716	5.61, 9.77	27.7	31.99	1.71
SBA-15-110 [§]	1	516	14.34, 17.2	30.9	35.68	2.42
SBA-15-120 [§]	1	464	14.35,	30.9	35.68	2.49
			19.85			
SBA-15-80 [§]	0.33	560	4.30, 3.91	24.32	39.63	0.92
SBA-15-80 [§]	0.16	631	5.3, 6.3, 3.9	15.19	17.54	0.86
SBA-15-80 [§]	0.08	600	6.34, 3.91	13.63	15.74	0.79

§ Indicates the Temperature for the Hydrothermal treatment; ‡ Estimated with the desorption branch of the isotherm, using the BJH method. Two given values indicate a bimodal pore size distribution.

Pure siliceous SBA-15 presents a narrow pore size distribution with an average diameter of 4.76nm. The pore size can be tuned by addition of TMB during the micellar formation, in a step previous to TEOS hydrolysis and polymerization. All mesoporous sieves exhibit a broader and bimodal size distribution, ranging from 5 to 20nm, in size. In addition, by increasing the hydrothermal temperature and pressure it



is possible to yield a material with a different morphology (micrographs obtained at 10kX magnification, bar length 1µm). SBA-15 presents an elongated club-like particle size

whereas higher temperature and pressure result in smaller round-like particles. Nitrogen adsorption and desorption isotherms are shown in the next figure (*right*). According to the classification made by IUPAC¹, all prepared materials exhibit a type IV isotherm, characteristic of mesoporous materials ranging from 2 to 50nm in size. Three well-defined regions can be identified: a) Monolayer formation at low relative pressure values (P_s/P_0); b) A slope change can be attributed to the capillary condensation and the P_s/P_0 value depends on the pore size, and c) The region encompassing values until 1.0 which can be attributed to the multilayer adsorption on the external surface area of the material. All materials feature an H1-type hysteresis loop, which is indicative of capillary pores with tubular symmetry. The Small Angle X-ray scattering curves (*left*) can provide information concerning the hexagonal arrangement of the prepared solids.



SBA-15 shows three well defined diffraction peaks in the low q interval, that can be assigned to the reflections of the (100), (110) and (200) planes, associated to the hexagonal structure, p6mm space group². As the amount of swelling agent increases, the intensity of the diffraction peaks is reduced and



is shifted to lower scattering vector values, suggesting materials with a lower degree of ordering. The lattice cell parameters shown in table 1 were estimated using this value. Nonetheless, all silicas exhibit high surface areas well above the values reported for amorphous silicates. Concerning the surface grafting of SBA-15, several reports can be found in the



literature on the functionalization of $SBA-15^3$ for specific chromatographic and adsorption purposes. Instead of the conventionally used alkyl silanes, here we present the formation of covalently attached monolayers of chlorodimethylphenylsilane, resulting in materials with contact angles over 130° , characteristic of very hydrophobic surfaces.

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1A – Nanostrategies for early diagnosis and treatment of FKBP12-related neurodegenerative amyloidosis

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Aims

Effective inhibitors of biomarkers for neurodegenerative pathologies were investigated with the twofold aim of developing a specific sensor nanotechnology able to detect traces of biomarker in the early phases of neurodegenerative disorders and formulate biocompatible nanovectors for the delivery of the biomarker-inhibiting drug in the therapeutic stage.

Results

The FKBP protein family is at the crossroad of several important metabolic pathways due to its central role in immunosuppression and cell proliferation as specific peptidyl-prolyl-isomerase (PPI) enzyme. Members of this family, and notably FK506 binding protein (FKBP12), are involved in Multiple Sclerosis, Amyotrophic Lateral Sclerosis and cancer [1]. Recent findings also evidenced that FKBP12 is over-expressed in early stages of neurodegenerative diseases such as Parkinson's and Alzheimer's and suggest a direct role of FKBP12 in the proliferation of amyloid fibrils [2].

Phase contrast microscopy images acquired for α -SYN, α -SYN/FKBP12 samples kept under magnetic stirring at 37°C for 30 days (Figure 1), clearly show that the aggregation of α -SYN is stimulated by FKBP12 binding.



Fig. 1: Phase contrast microscopy images of a-SYN (a), a-SYN/FKBP12 (b), and a-SYN /FKBP12/ElteN378 (c). CLSM images and spatially-resolved emission spectrum for CR.

The amyloid fingerprint of such structures, evidenced by the specific emission of Congo Red at 597 nm, was confirmed by means of Confocal Laser Scanning Microscopy combined with spatially resolved fluorescence.

A new class of nanomolar inhibitor for FKBP12 was recently designed and synthesized on the basis of theoretical modeling of the minimal structural requirements for the pharmacophore binding to the FKBP pocket: ElteX compounds [3,4].

The strong binding of ElteN378 to the protein was found to dramatically affect the amplification of fibrils proliferation as shown in fig.1 d for the system α -SYN/FKBP12/ElteN378. Addition of ElteN378 to α -SYN/FKBP12 system results in the disappearance of the extended network of fibrillar aggregates replaced by smaller and amorphous structures. Confocal Laser Scanning Microscopy combined with spatially resolved emission proved that such amorphous structures do not contain β -amyloid motifs.

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1A – Surface engineering of nanostructured oxide systems for solar energy conversion

S. Vitale, G. Zappalà, N. Tuccitto, A. Torrisi, F. Ronconi, M.P. Santoni, S. Campagna, A. Licciardello

Aims

The work is aimed to develop methodologies for anchoring of functional molecules on transparent (semi)conducting oxide surfaces, for perspective applications in solar energy conversion devices. The anchoring must be robust, in order to ensure a long lifetime of the device and, at the same time, it must permit the molecule-to-oxide charge injection.

Results

The strategy, sketched in the scheme, involves the preliminary stepwise surface modification [1] based on the chemistry of zirconium phosphates/phosphonates (ZP-priming), consisting in the deposition on a zirconium-phosphate layer directly at the hydroxylated oxide surface, that allows the subsequent anchoring of a phosphonate-functionalised molecule.



The strategy was successfully applied to nanostructured, micrometres-thick TiO2 and SnO₂ substrates. The efficacy of the method in providing a uniform priming along the entire nanostructured layer was studied and assessed by ToF-SIMS depth profiling measurements.[2] ZP-TiO₂ and ZP-SnO₂ films were subsequently used as substrates for the preparation of photoactive electrodes with perspective application in dyesensitised cells for solar energy conversion. The ZP treatment provides a suitable anchoring platform for the sensitisation with photoactive dye RuP (a ruthenium tepryridyl-triazin complex bearing a phosphonic group). ToF-SIMS depth profiles demonstrate (as shown the uniformity Ru signal across the nanostructured film) that the sensitisation involves the whole thickness of the oxides layers, while UV-Vis spectroscopy data show the presence of a greater amount of adsorbed layer molecules compared with the conventional impregnation methods. Moreover, the anchoring obtained through the ZP methodology appears to be bore stable in accelerated lifetime tests. Finally, photoelectrochemical measurements (namely JV characteristics upon irradiation) demonstrate that the presence of the zirconium-phosphate-phosphonate layer at the interface between oxide and dye molecule does not negatively affect the

dye-to-oxide charge injection. These data show the photoelectrochemical properties are maintained and no detrimental effect occurs, and in some cases the electrode performances seem to be even improved from the ZP-treatment.



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1A – Electrical investigation of molecular wires

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Aims

Understanding the charge transfer and charge transport mechanisms is of central interest in chemistry, physics and biology, because of their crucial role in numerous processes involving molecular, supramolecular and biological systems. Here we have used a coordination chemistry strategy to fabricate Fe(II)-bis(terpyridine) conductive molecular assemblies by means of layer-by-layer growth on gold substrate, with the aim to get insights into the charge transport mechanisms of these ordered nanostructures.

Results

Supramolecular chemistry can be very useful in obtaining a wide range of system with different properties. In this particular context, polymetallic (supramolecular) complexes can be used as models for the study of electron transport mechanism in a molecular junction. Assemblies of molecular wires mased on Fe-bis(terpyridine) complexes have been grown on gold surfaces via a self-assembling stepwise method involving direct coordination reactions [1-2] at the sample surface, in order to study their electrical behaviour using the conductive AFM technique.



As easily observed, current decreases with the increasing number of layers. In particular, the dependency of the current at a fixed bias value as a function of the thickness of the multilayer shows a linear decrease. The same behavior is observed by plotting the resistance values: a linear increase is observed with increasing thickness, that is typical of ohmic conductors.

Moreover, by using the equations $I = I_0 e^{-\beta L}$ and $R = R_0 e^{\beta L}$ respectively for the current values at a fixed voltage and for low bias resistances, it is possible to determine a β value, that in our case is estimated to be $\beta = 0.058 \pm 0.006$ Å-1. This value provides unambiguous evidence for the existence of a hopping charge transport mechanism.[3]

The log-log plot of the I-V characteristics (d) provides a mean for understanding if is a change in transport regime as a function of the voltage is occurring. In the case of shorter wires, less than 3.5 nm long, the electrical data indicate an ohmic conduction mechanism. On the contrary, longer wires (> 4 nm) exhibit a transition in transport mechanism at certain voltages, to a regime in which the current is roughly following a quadratic dependence on the bias, indicative of a space charge limited current (SCLC) regime.

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1B – Rheology and Rheo-NMR-Imaging of lecithin-based viscoelastic solutions.

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Aims

Despite the great deal of results available on the complex shear flow of aqueous wormlike micellar (WM) systems, which require the presence of cosurfactants or counter-ions, less attention has been given to the rheological response of oil continuous WM systems, which offer the advantage to neglect the electrostatic interaction played by salt concentration. To fill this gap, NMR micro-imaging and NMR velocimetry techniques, in combination with bulk rheology, have been used to understand the flow behaviour of reverse nonionic wormlike micelles stabilized by phospholipids (lecithin) in the organic solvent cyclohexane (lecithin organogel) where the amount of dispersed water corresponded to ten water molecules *per* lecithin molecule.

Results

Experimental flow curves at various lecithin volume fractions $\phi = 7$, 14 and 28 wt %, were characterized by the presence of stress plateaus up to an upper shear rate limit $\dot{\gamma}_{high}$, which signed the end of the coexistence of the isotropic-nematic shear-banding regime (see Figure 1).



For applied shear rates $\dot{\gamma}$ within the stress plateau, ¹H-NMR-density weighted images of 1 mm thick 2D slices of the sample within the cell gap acquired with the Gradient Echo Fast Imaging (GEFI) pulse sequence, revealed a new phase nucleating inhomogeneously at the inner rotating cylinder (Figure 2). In steady state conditions, the shear induced (nematic) phase developed periodic fluctuations in space whose Fourier Transform analysis indicated that the perturbed flow consisted of a vortex-type pattern with wavelength $2\pi/k$, k being 3 mm⁻¹ and 4 mm⁻¹, respectively, for $\dot{\gamma} = 0.028 \text{ s}^{-1}$ and $\dot{\gamma} = 0.07 \text{ s}^{-1}$.

Elastic instabilities, generally observed in polymer solutions, may be responsible for the nucleation of Taylor-like vortices, developing along the neutral axis with a characteristic length-space frequency (Figure 2).

In addition, slippage phenomena have been found in flow regimes consistent with a full shear-induced nematic state.



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1B – Phyto-Liposomes as biocompatible carriers for natural drugs

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Aims

Silybin, the main component of silymarin, is a polyphenolic bioactive natural product extracted by the milk thistle plant *Silybum marianum*. Silybin possesses many health-promoting activities, such as antioxidation, anticancer and hepatoprotective. However, the benefits are curtailed by its extremely poor water solubility, which limits its bioavailability and therapeutic efficiency. Currently, the efficacy of natural extracts may be improved through their incorporation into liposomes, thanks to their versatility to control the delivery of the loaded drug to the target. Here, we developed a formulation based on the incapsulation into liposomes of a silybin-phospholipid complex, commercially available with the trade name SiliphosTM, to yield a new type of supramolecular aggregates, also called *Phyto-Liposomes*. The hepatoprotective activity of new formulation was finally tested on human hepatoma cell systems supporting HCV replication and infection.

Results

First, we set up a simple preparation protocol through the reverse-phase evaporation method and investigated the physico-chemical properties of the obtained liposomial suspensions. A careful investigation of host-guest interactions was carried out by performing UV–vis (A) and spectrofluorimetry (B) experiments in non-polar solvents (1:1 mixture of DMSO and benzene), to probe the influence of phospholipids on the electronic properties of silybin and its propensity to engage H-bonding with the lipid headpolar groups (SIL=silybin; SiliphosTM = 1:1 complex silybin-phospholipids).



Then, it was demonstrated the ability of phyto-liposomes to be internalized in human hepatoma Huh7.5 cells, being 2.4 fold more efficient than the plant extract silybin. Finally, the new formulation was tested on cell systems supporting HCV replication and infection, and its spectrum of pharmacological activities was compared with that of the active principle dissolved in DMSO, revealing a three hundreds fold more potent pharmacological activity.



Moreover, it was assessed that phyto-liposomes were unable to impair the integrity of viral particles, they had no inhibitory effects on HCV replication regardless of genotype and no competition with HCV for Chlatrin-dependent endocytosis mechanism was observed.

The maximum inhibition effect was obtained when phyto-liposomes and viruses supernatant were simultaneously added to cells, whereas no effect on previously infected cells could be detected. Considering that phyto-liposomes were able to inhibit HCV infection, they could be administered soon after the liver transplant, presumably without significant side effects. This perioperative strategy could prevent circulating or extrahepatic virions remained in the recipient to re-infect the transplanted liver, event that usually occurs within few hours after liver transplant.

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1B – Formulation of liposomes functionalized with specific protein and effective in targeting highly proliferative cells

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Aims

Liposomes, used for decades to improve the therapeutic index of new and established drugs, have advanced with the insertion of active targeting.

Results

Doxorubicin-loaded liposomes functionalized (Dox-FL) with the specific target protein, that in this case preferentially binds glycans with alpha-1,2-linked fucose, have been synthesized. A target protein was introduced into the lipid bilayer of DOPC/DOPE liposomes. Functionalization of liposomes with protein did not alter size, surface charge, ζ -potential or overall structure of the vesicles.

By confocal laser microscopy we analyzed the presence and localization of *the active target* and uptake processes in two cancer cell lines. We then constructed doxorubicin-loaded functionalized liposomes. Intracellular delivery of the drug was determined *in vitro* and *in vivo* by confocal and electron microscopy.



Fig. 1: Uptake for 36 hours of Dox-FL (A) and Dox-L (B) in cancer cells of the DU145 line by confocal microscope (A and B).

We confirmed the specific localization of the binding sites and the uptake mechanism in the two cell lines and determined that functionalized liposomes loaded with doxorubicin greatly increased intracellular delivery of the drug, compared to unmodified doxorubicin-loaded liposomes. The Dox-FL mechanism of entry and drug delivery was different to that of Dox-L and other liposomal preparations. Dox-FL entered the cells one by one in tiny tubules that never fuse with lysosomes. Dox-FL injected in mice with melanoma specifically delivered loaded Dox to the cytoplasm of tumor cells.



Fig. 2: Cellular uptake for 24 hours of Dox-FL *in vivo*. Fluorescence microscopy images of two sections of the melanoma tumor and one section of heart, showing the localization of Dox upon the intravenous administration of 100 μ l of liposomes.



Fig. 3: 600 MHz NMR proton spectrum in D_2O (range 0-4.5 ppm) for: A) empty liposome; B) Dox-FL liposome and C) Doxorubicin (Dox)

To evaluate the interaction processes in liposome systems (Dox-FL, Figure 3B), the ¹H spectrum of doxorubicin in D₂O (figure 3C) and pure liposome (Figure 3A) were recorded. The observed signal broadening was associated with the interactions with the target protein and doxorubicin. Since it was not possible to detect preferential broadening of the polar heads or the alkyl chain signals, this effect was attributed to growth of the overall aggregates. The inclusion of specific target in a liposome formulation is a fundamental step for improving the loading and transport processes of doxorubicin. The NMR spectrum of

functionalized liposomes showed that the protein does not substantially modify the structure of the liposome.

Liposome functionalization with specific target protein promises to broaden the therapeutic potential of liposomal doxorubicin treatment, decreasing non-specific toxicity.

Doxorubicin-FL functionalized liposomes promise to be useful in the development of new cancer chemotherapy protocols.

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1B – Effect of Resveratrol on Platelet Aggregation by Fibrinogen Protection: NMR, IR and SEM experiments

C. Bonechi, S. Lamponi, A. Donati, G. Tamasi, M. Consumi, G. Leone, C. Rossi, A. Magnani

Aims

The ability of resveratrol in preserving fibrinogen from denaturation and platelets from aggregation was studied using combined spectroscopic and biological analyses.

Results

Resveratrol (RSV), an antioxidant found in red wine, is able to decrease the incidence of coronary heart disease. RSV blocks platelet aggregation by the protective action characteristic of antioxidant compounds. We investigated the effect of RSV in inhibiting both platelet adhesion and aggregation and fibrinogen conformational changes promoted by epinephrine, using complementary experimental techniques.

Nuclear magnetic resonance and infrared spectroscopies were used to investigate the protective effect exerted by resveratrol toward fibrinogen (FBG) in presence of epinephrine (EP) which, as well known, induces strong variations in the secondary structure of fibrinogen when reaching the stress level concentration.

The protective effect of RSV towards FBG was evident by both spin nuclear relaxation experiments, determining the thermodynamic equilibrium constants of FBG-EP interaction and infrared measurements, analyzing the EP-induced conformational changes of FBG. In particular, the spin nuclear relaxation showed that the strength of the interaction between epinephrine and fibrinogen was strongly decreased by the presence of resveratrol (Figure 1A). These data were confirmed by IR spectroscopic measurements that emphasize the protective effect of the antioxidant compound towards fibrinogen. The infrared data, in fact, showed that fibrinogen was not denatured by the interaction with epinephrine in presence of resveratrol (Figure 1B).

Resveratrol inhibits the protein interaction with the hormone and thus reduces the degree of platelet adhesion and aggregation. SEM analysis, in fact, revealed that the presence of resveratrol completely inhibited the platelet aggregation and the degree of platelet adhesion decreased by increasing the resveratrol concentration (Figure 2). Moreover, resveratrol was also able to reduce the percentage of platelet aggregation in PRP.



Fig. 1: A) Reciprocal of selective relaxation rate enhancements in relation to epinephrine concentration with and without RSV; B) Amide I and Amide III deconvoluted difference FTIR-ATR spectra of: native FBG (red spectrum), FBG-EP system (blu spectrum), FBG-EP-RSV system (pink spectrum) in normal saline solution



Fig. 2: Scanning Electron Microscopy images of platelets after contact with: a) EP 15 mM; b) EP 15 mM and RSV 60 mM.

The protective properties of resveratrol towards fibrinogen from the denaturant activity of epinephrine can be explained on the basis its ability to bind the catecholamine.

Our combined results pointed out that resveratrol is able to protect both fibrinogen and platelets from the denaturant and aggregating action of epinephrine at the stress level concentration.

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1B – Effect of quercetin-loaded liposomes on induced oxidative stress in human spermatozoa

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Aims

The study of natural compounds with antioxidant properties is appealing since it can offer the possibility of therapeutic options for male infertility and the development of new strategies of media supplementation in vitro used for semen handling. A strategy to circumvent the poor polyphenols bioavailability is to load these compounds into liposomes.

Results

We evaluated the in vitro effects of quercetin (Q) and Q-loaded liposomes on motility, viability and chromatin integrity of swim-up selected human sperm. Antioxidant power was assayed against tert-butylhydroperoxide induced lipid peroxidation (LPO) using C11-BODIPY581/591 fluorescentprobe and transmission electron microscopy. Q-loaded liposomes showed decreased toxicity for sperm motility and viability and increased DNA damage compared to quercetin. The percentage of sperm with fluorescence, marker of LPO, was decreased in samples incubated with quercetin vs Q-loaded liposomes (P < 0.001). The ultrastructure of acrosomes and membranes was preserved with quercetin, whereas Q-loaded liposomes did not prevent membrane injury.



Fig. 1: Mean and SD of the percentages of viable and progressive motility sperm treated with Q-loaded liposomes and Q at different concentrations.

Respect to free Q, Q-loaded liposomes showed decreased toxicity for sperm motility and viability, increased genotoxicity, especially if used at high concentrations, and they were not active against induced LPO in human sperm. The different behavior of Q and Q-loaded liposomes could be explained by a different mechanism of action: Q may act outside the cell modulating sperm motility and counteracting LPO at plasma membrane level, the liposomes plausibly deliver Q inside the sperm cell for this reason the antioxidant effect of Q on induced LPO is decreased and the negative effect on DNA is evident.

Liposome Composition	Size (nm)	P.I.	Zeta potential (mV)	Encapsulation Efficiency (EE) %
DOPC/DOPE	105 ± 15	0.16	-11 ± 5	
DOPC/DOPE + Q (1:1)	113 ± 10	0.20	-19 ± 7	18.9 ± 5.3
DOPE/DOPA	109 ± 13	0.17	-37 ± 2	
DOPE/DOPA + Q (1:1)	125 ± 21	0.21	- 32 ± 5	14.2 ± 1.9
DOPE/DOTAP	115 ± 12	0.15	48±5	
DOPE/DOTAP + Q (1:1)	124 ± 15	0.19	50 ± 9	15.6 ± 1.5

Table 1. Size, surface charge and encapsulation efficiency of Q-free liposomes and Q-loaded liposomes.

Results of the size distribution and surface charge values of Q-free liposomes and Q loaded liposomes are presented in Table 1.In all cases, there was a slight increase in liposome mean diameter when Q was incorporated. The difference in the mean diameter of Q-free liposomes and Q loaded liposomes was small indicating that Q can be well loaded in the lipid bilayers. The low polydispersity indexes (P.I.) showed that the liposomes were not altered by the interactions with Q.

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1B – In vitro assays for the "ORAC" classification

M.C. Baratto, M.L. Parisi, M. Al Katib, R. Basosi, R. Pogni

Aims

Scavenger and antioxidant activity of extracts and fractions using in vitro assays are carried out through EPR spectroscopy and spectrophotometrically.

Results

Antioxidants act against "free radicals" in order to scavenger them. The determination of antioxidant activity of single components or extracts is performed through assays (ORAC) that measure the capability of such molecules to reduce the presence of reactive radicals, mainly oxygen ones, such as ROS.

EPR (electron paramagnetic resonance) spectroscopy is a crucial technique for the analysis, determination and quantification of antioxidant activity. It is specific for the study of paramagnetic species such as radicals. As free radicals are very labile and difficult to be detected spectroscopically at room temperature, the EPR-spin trapping technique is a powerful approach in order to trap radical species and form stable adduct to be studied at room temperature. EPR spectroscopy is a non destructive technique which gives a direct analysis of the free radical quantity and an indirect measurement of the antioxidant activity. Antioxidant activity of food, extracts or single molecules is monitored and quantified through the reduction of stable radical signal present in the sample understudy.

The research carried out by the University of Siena started in 2003 with the antioxidant activity study of some galloil quinic extracts from Pistacia lentiscus leaves and some spectrophotometric and spectroscopic EPR assays were developed towards DPPH and ROS radicals.



Then the study was focused on the biochemistry of Olea europea leaves submitted to high light and salinity and the defence of leaves against oxidative damages due to water stress and salinity.

Recently antioxidant properties of polyphenolic fractions of Cistus incanus leaves and of an extract from Consalida maggiore (Symphytum Officinale) root have been tested and are still under study.



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1B – Interaction of Antimicrobial Peptides with lipid membranes

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Aims

The aims of this work is to study the interaction of bioactive antimicrobial peptides with phospholipids membranes combining several spectroscopic techniques (i.e. Circular Dichroism, Fluorescence Emission, Site Directed Spin Labeling – Electron Paramagnetic Resonance) in order to clarify various features that regulates the mechanism of this interaction.

Results

Antimicrobial peptides (AMPs) are an essential part of innate immune defence system against microbial infection. Naturally occurring AMPs are basic peptides composed of 12-50 aminoacids that are ubiquitously distributed throughout all kingdoms of life. AMPs display a broad spectrum of antimicrobial activity against both Gram-negative and positive bacteria, fungi and enveloped viruses. Importantly, they retain activity against antibiotic-resistant strains and do not readily elicit resistance. AMPs base their capability to kill pathogens on the perturbation and the disruption of membrane cell wall.

We investigated in details the mechanism of peptide-lipid interaction and the relative factors that influence the partition into lipid bilayer of two human antimicrobial peptides, human neutrophil peptide 1 (HNP-1) and cathelicidin LL-37, which exhibit a synergistic action against various pathogens *in vivo*.

We find that the defensin HNP-1 interacts with phospholipids mimicking Gramnegative inner membrane adopting a "spanning-mode" into a lipid bilayer only reaching a specific threshold concentration represented by the 1:20 peptide:lipid molar ratio (Fig.1). The residue Arg-14 plays a fundamental role on the HNP-1 partition: in fact, replacing this residue with less cationic aminoacids altering the penetration of peptide into model membrane. Another limiting factor for HNP-1 activity is represented by cysteines connectivity. The reduction of disulphide bonds does not compromise the partition of peptide into model bacteria membrane expanding the applicability of HNP-1 on therapeutic treatment of infections. In addition, an analysis on the interaction of this peptide with model mammalian membrane provided that HNP-1 does not posses a relevant toxicity against eukaryotic lipid bilayer.

Another study is based on the mechanism of action of human AMP LL-37 against model bacteria membranes versus host cell model membranes. In this context, antimicrobial peptide LL-37 and two variantswere studied in the presence of model membranes with different lipid compositions andcharges. The investigation was performed using an experimental strategy that combines thesite-directed spin labeling-electron paramagnetic resonance technique with circulardichroism and fluorescence emission spectroscopies. LL-37 interacts with negatively chargedmembranes forming a stable aggregate, which can likely produce toroidal pores until theamount of bound peptide exceeds a critical concentration. At the same

time, we have clearly detected an aggregate with a higher oligomeric degree for interaction of LL-37 with neutral membranes. These data confirm the absence of cell selectivity of the peptide and a more complex role in stimulating host cells.



Our studies provide new insights on the mechanisms of interaction with phospholipids membranes for defensin HNP-1 and cathelicidin LL-37. Principally, we expand the knowledge on AMPs, supporting the applications of these biologic compounds as possible substitutes of common antibiotics on therapies for the treatment of infections. Since both HNP-1 and LL-37 peptides are related to specific diseases, such as cystic fibrosis, our analysis supply information to understand and solve the processes that leads to the inception of these pathologies.

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1B – EPR investigations of enzyme-ligand complex in copper containing proteins

M. Al Khatib, M.C. Baratto, R. Pogni, R. Basosi

Maher Al Khatib's PhD project is focused on the development of electron paramagnetic resonance methodologies. The central part of the work is oriented toward the implementation and application of a various range of pulsed EPR experiments to substrate of biological, biochemical and industrial interest, such as enzymes and metalloproteins. These experiments, along with the classical continuous wave (cw) EPR techniques, will provide knowledge of the structure and dynamics of the paramagnetic centers in such systems.

The pulsed experimental setup is based on a SuperQ-FT bridge which is able to generate Q band microwave pulses on the nanosecond timescale. The continuous wave experimental setup allows Q, X and S band measurements for multifrequency studies. It is important to notice that the project promotes a strong interaction between the experimental part of the work and the theoretical knowledge needed to perform it successfully. Recently, low temperature cw experiments have been performed on two new enzymes of possible industrial interest: a fungal laccase and a tyrosinase from Algerian desert soil isolates. Both these enzymes share a pair of antiferromagnetically coupled Cu(II) ions into their catalytic site ("type3" copper center, T3), even if laccases in contrast to tyrosinases, use also two other distinct mononuclear Cu(II) ions to exert their catalytic activity: the so called type1 (T1) and type2 (T2) copper centers, both EPR active (Fig. 1). In presence of exogenous ligand, the T3 antiferromagnetic coupling can be broken, making the T3 site suitable for EPR analysis.



Fig. 1: Schematic representation of the overall catalytic mechanism in laccases. Four copper ions are present. The T3 site (yellow) is the one present both in laccases and tyrosinases.

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1B – Loading, protection and release of hydrophylic molecules entrapped in liposome based multishell nanocapsules

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Aims

Loading and release behaviour of hydrophilic molecules as function of pH and wall thickness.

Results

Compartmentalized systems produced via the layer-by-layer (LbL) self-assembly method have been produced by alternatively depositing alginate and chitosan layers onto cores of liposomes. The possibility of encapsulating and releasing molecules from this type of nanocapsule was demonstrated by loading high (FITC-dextran 20, 40, 70 kDa) and low molecular weight (Rhodamine B) molecules into the liposome core. The release of the loaded molecules from the nanocapsule was demonstrated after liposome core dissolution.

The combination of dynamic light scattering (DLS), ζ potential, and transmission electron microscopy (TEM) techniques provides detailed information on the stability, dimensions, charge, and wall thickness of these polyelectrolyte globules. TEM microphotographs demonstrate the presence of nanocapsules with an average diameter of below 300 nm and with a polyelectrolyte wall thickness of about 20-25 nm. Even at low molecular weight, the nanocapsules appear to be appropriate for prolonged molecule compartmentalization and protection. By means of the Ritger–Peppas model, non-Fickian transport behaviour was detected for the diffusion of the entrapped molecules through the polyelectrolyte wall.

Values of the diffusion coefficient were calculated and yield useful information regarding chitosan/alginate hollow nanocapsules as drug-delivery systems. The influence of the pH and of the wall thickness on the release properties were also considered. The results indicate that vesicle templated hollow polyelectrolyte nanocapsules show great potential as novel controllable drug-delivery devices for biomedical and biotechnological applications.

time/min pH7.4 pH4.5 0 60 120 180 240 300 0 3 number of Tayers 7 Fig.: (A) Release profiles of FITC-dextran 20, 40, 70 kDa at pH 7.2 and 4.5 from capsules made of 5 polyelectrolyte layers, (B) Release behavior of FITC-dextran extrapolated from experimental data according to the Ritger–Peppas model. (c) Release profiles of Rhodamine B from bare liposomes and from nanocapsules with three, five and seven layers at pH 7.2. (D) Release behavior of Rhodamine B extrapolated from experimental data according to the Ritger–Peppas model. The line drawn in the graphs B and D indicates the boundary between the values of n typical of Fickian (<0.43) or non Fickian diffusion (>0.43).

pH 7.4

nH 4 4

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1B – Coumarin derivative for sensing application: nucleotides identification using a micellar system

F. Cuomo, A. Ceglie, C. Caltagirone, S. Murgia, F. Lopez

Aims

Easy and controlled the use of a novel lipophilic coumarin derivative in aqueous environment for sensing application.

Results

The recognition of nucleotides is of crucial importance because they are the basic constituents of nucleic acids. The present study is focused on the selective interaction between a novel amphiphilic fluorophore containing coumarin and imidazole, CI (1methyl-3-(12-((2-oxo-2H-chromen-7-yl)oxy)dodecyl)-1H-imidazol-3-ium bromide), and different nucleotide-monophosphates (NMPs). It was supposed that the solubilisation of the low water soluble CI in a micelle system of hexadecyltrimethylammonium chloride (CTAC) would make the coumarin moiety of CI available to the interaction with the water-soluble NMPs. Changes in CTAC critical micelle concentration suggested that CI strongly interacted with the host cationic surfactant, thus forming a positively charged interface enriched with coumarin able to interact with the anionic NMPs. Steady-state fluorescence quenching revealed that CI/CTAC system was capable of distinguish between purine- and pyrimidine-based nucleotides. A modified Stern-Volmer equation permitted the use of a quenching model that accounted for the possible interactions between the micelles and the nucleotides. The data analysis allowed calculating selective parameters that differentiated according to the type of nucleotide either at 25 or 50 °C. Our results established the utility of the novel coumarin derivative fluorophore, supported by the simple and suitable micellar systems, as a tool for DNA sensing applications.



Fig. 1: Normalized fluorescence intensities at 392 nm (λ exc = 325 n m) of CI solubilized in CTAC micellar solution. as function of nucleo-tide concentrations (AMP, GMP, UMP, TMP, CMP) (left). Schematic representation of the CI/CTAC system and nucleotide mono-phosphates (left).


Fig. 2: Fitting of the fluorescence quenching data to the modified Stern-Volmer equation at 25 and 50°C. The intercepts of the straight lines are in agreement with the differences in terms of probe accessibility and differentiate between purine and pyrimidine based nucleotides.

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1B – Cubosomes and hexosomes in theranostic nanomedicine

S. Murgia, C. Caltagirone, V. Lippolis, M. Monduzzi

Aims

We explored the potential of monoolein-based non-lamellar liquid crystalline nanoparticles, namely cubosomes and hexosomes, as theranostic tools.

Results

We proved that cubosomes and hexosomes allow for the encapsulation of antineoplastic poorly water-soluble drugs (quercetin, camptothecin, and docetaxel) and that the presence of such drugs within the lipid bilayer did not affect the nanostructural and morphological characteristics of the nanoparticles. Furthermore, we observed the superior cytotoxic ability of docetaxel towards HeLa cells when embedded in the cubosomes matrix with respect to its use as a free drug. Similarly, we demonstrated these nanocarriers can be simultaneously coupled with fluorescent imaging agents still preserving the original physicochemical features of pristine cubosomes and hexosomes nanoparticles. In addition, also the photophysical properties of the imaging agents, critical for the fluorescence optical imaging, are retained in the colloidal systems. Sometimes, these properties were extremely helpful for understanding the fluorophore localization in the nanoparticle (solvatochromism). In the frame of possible applications in cancer treatments, we made cubosomes and hexosomes actively targeted by decorating their surface with folic acid. Thanks to this modification the uptake of targeted cubosomes in HeLa cells considerably increases with respect to pristine cubosomes.



A detailed study of changes occurring in HeLa cells, when exposed to treatment with monoolein-based cubosomes, was conducted. Such investigation is of primary importance within the context of biomedical applications. It was observed that the uptake of cubosome formulations induced modification of the cell lipid profile, lipid droplet accumulation, mitochondrial hyperpolarization and mitochondrial ROS generation. Remarkably, these modifications did not cause significant toxicity in HeLa cells. Finally, to evaluate the potential of cubosomes as diagnostic tools in diabetes and pancreatic β -cell transplantation, a newly synthesized hydrophobic dye was entrapped with their lipid bilayer. Rat pancreatic β -cells readily took up the cubosome nanoparticles, as revealed by in vitro internalization tests, and flow-cytometric analyses confirmed the persistence of the fluorescence for up to 24 hours. All these results strongly encourage further investigation of non-lamellar lipid liquid crystalline

nanoparticles in thereanostic nanomedicine, and for pharmaceutical applications in general.

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1B - Poly(vinyl alcohol)-based microgels prepared through salting out: rationalising the aggregation process

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Aims

Rationalisation of the aggregation process of poly(vinyl alcohol) in the presence of sodium chloride, thermodynamical characterization of polymer solutions and structural properties of PVA particles obtained through salting-out.

Results

Poly(vinyl alcohol) (PVA) is a biocompatible water-soluble polymer of great interest thanks to its large-scale applications as a material for drug-delivery systems or for building sensors and membranes with selective permittivity. The cryogenic route is one of the most studied and widely employed techniques for the preparation of PVA physical hydrogels [1]: the advantages of such gels is the absence of toxic chemicals for their preparation and the consequent possibility to obtain a completely eco-friendly product [2].

In this work we propose a new route for the preparation of PVA-based microgels through the salting-out effect: after a screening of different salts belonging to the Hofmeister series, sodium chloride represented the best cosmotropic species to use in order to favour the polymer aggregation over a reasonable time-scale.

The thermodynamic properties and the kinetics of the aggregation process were deeply studied through a combined Dynamic Light Scattering (DLS), Static Light Scattering (SLS) and Small Angle Neutron Scattering (SANS) study, which allowed rationalising how such process is influenced by different parameters like salt molality, polymer concentration and time from the preparation (fig. 1).

Moreover, we were able to shed light on the structural and morphological properties of PVA particles, showing the role of the salt in the aggregation process and its effect on the supramolecular organization. In particular, we determined the molecular weight and the radius of gyration of the aggregates and we estimated the packing degree of polymer chains within the aggregates, strongly influenced by the time and the salt concentration.



Fig. 1: PVA 1% wt, NaCl 2 mol kg-1: study of the evolution of hydrodynamic radii over time by DLS (panel A); Zimm plot obtained from SLS measurements (panel B); SANS results at different times from the preparation (panel C).

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1B - Neuroprotective effect of poly-unsaturated fatty acids: structure, dynamics and interaction with amyloid peptides of Omega-3 containing lipid bilayers

A. De Santis, G. D'Errico, L. Paduano

Aims

Evaluation of the Effect of Docosahexaenoic Acid on the dynamics and structures of lipid bilayers and on the interaction with peptides.

Results

Among the Omega-3 Poly Unsaturated Fatty Acids (PUFA), DocosaHexaenoic Acid (DHA) is the most important one found in cell membrane; indeed it has a pivotal role in the prevention of cardiovascular diseases and cancer and exerts a strong neuroprotective effect [1,2].

Omega-3 fatty acids were proposed to alter the physicochemical features of the membrane, once converted to phospholipids, and/or to segregate cholesterol molecules in liquid ordered domains (L_o), typically associated to the lipid rafts [3]. However, their mechanism of action is still elusive.

With the aim to understand the functional role of DHA, we investigate the influence of dipolyeneOmega3-PC (one of the possible phospholipids containing DHA) on the micro-structural properties and phase behaviour of a lipid membrane composed by 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC), Cholesterol (Chol) and Omega3-PC. The physico-chemical techniques employed are Electron Spin Resonance (ESR) spectroscopy with the spin-labelling approach and Neutron Reflectivity (NR).

Moving from the characterization of the lipid system, we attempt to rationalize the PUFA effect on peptide/lipid interaction, focusing on the neuroprotective effect of Omega3-PC. Through a combined ESR and Circular Dicroism (CD) study of the interaction between the Alzheimer peptide $A\beta$ -(1–42) and a PUFA containing lipid bilayer, we show that the higher the Omega-3 lipid content the higher the membrane-peptide interaction (Figure 1) and that this interaction effectively prevent peptide aggregation. These results suggest that $A\beta$ -(1–42) selectively interacts with DHA containing membranes and may provide hints for mechanism and therapy of Alzheimer disease [4].



Fig. 1: Variation of the order parameter, S, in the inner apolar region of the bilayer over time, upon A β 1-42 peptide addition, for three lipid bilayers with increasing amount of Omega3-PC.

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1B – Characterization of protein-NPs interaction and development of aptamer functionalized NPs

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Aims

Development of different nanoparticles as selective therapeutic and theranostic agents for biomedical applications.

Results

We investigated the interaction between superparamagnetic nanoparticles (NPs) bearing a double layer of oleic acid/oleylamine and the lysophosphatidylcholines 18LPC with different model and serum proteins, including hen egg white lysozyme, human transferrin and human serum albumin (HSA).

Effect of NPs on the small model protein lysozyme where negligible, with no effect on thermal stability of secondary and tertiary structure up to 2 days of incubation. Furthermore no clear indication of the formation of a protein corona was obtained. In the case of human transferrin, effect on the tertiary structure of the protein and formation of protein-NP aggregates where observed only upon 24 h when a 1:50 NPprotein molar ratio was investigated. Analysis on the HSA-NP system are in progress. Results collected up to now indicate a high biocompatibility of the NP system encouraging its use for biomedical applications.

At the same time we started a research line aimed at functionalize different NPs with DNA aptamer able to recognize an important biomedical target and to exert a therapeutic effect. We were able to functionalize silica NPs with a modified thrombin binding aptamer obtaining a powerful anticoagulant agent. Now we are designing hydrophobically modified aptamers to be bound on the double layer of the superparamagnetic NPs.

1B – Effect of Cardiolipin on Lipid Bilayers

A. Luchini, G. Vitiello, L. Paduano

Aims

Characterization of the effect of Cardiolipin on the structure of supported lipid bilayers in the presence of divalent ions (i.e. Ca^{2+}).

Results

The effect of CL on lipid bilayers composed by POPC and POPE in the presence and in the absence of Ca²⁺ ions has been preliminary characterized by means of Quartz-Crystal Microbalance with Dissipation monitoring (QCM-D). In these experiments the vesicle suspension were prepared in phosphate buffer (pH=7.4) with 130 mMNaCl and KCl, to which eventually 1mM CaCl₂ was added. The frequency shift (ΔF , evaluated from the quartz support harmonic n=3) for POPE/POPC system in the presence of 1mM CaCl₂ corresponds to -28 and indicates the formation of a lipid bilayer. On the other hand, in the POPE/POPC/CL system, as well in the presence of 1mM CaCl₂ (Figure 1, panel a), the ΔF is -35 and the different harmonics are not well superimposed (the sample does not oscillate in phase with the support). These evidences suggest that CL is responsible for a different organization of the phospholipids. The effect of 1mM CaCl₂ on lipid bilayer prepared with POPE, POPC and CL (40/40/20 w/w/w) was investigated by means of Neutron Reflectometry measurements (Figure 2). Even at this low concentration of CaCl₂ there is a detectable effect of the presence of the Ca²⁺ ions in all the explored contrasts (D₂O, H₂O and SMW). By the comparison of the experimental data it is visible a change in the shape of the curves around 0.05 and 0.16 A⁻¹ that can be interpreted in a thickening of the bilayer in presence of calcium salts. All together the collected results indicate that there is an interesting effect of CL on the organization of POPE and POPC lipids both in the presence and in the absence of CaCl₂; this effect requires further investigation planned in the future experiments.



Fig. 1: QCM-D data collected for POPE/POPC/CL (40:40/20 w/w/w) in PBS + 1mM CaCl₂ (panel a); NR data collected during the test on FIGARO for the POPE/POPC/CL in H₂O buffer (blu curve) and POPE/POPC/CL in H₂O buffer +1mM CaCl₂ (red curve).

1B – Bioinspired eumelanin-based nanomaterials for antimicrobial applications

G. Vitiello, A. Pezzella, G. D'Errico, M. Varcamonti (Department of Biology, University of Naples "Federico II", Naples, Italy), G. Luciani

Aims

Design, synthesis and physico-chemical characterization of hybrid Eumelanin- TiO_2 nanomaterials with antimicrobial properties.

Results

Organo-inorganic hybrids, made by coupling inorganic phases to organic molecules, not only combine the often dissimilar characteristics of inorganic and organic components into one material, but often show unique and peculiar properties. This provides the opportunity to invent a huge set of new multifunctional materials with a wide range of applications in the fields of energy, health and electronics.

Herein, we provide a novel synthesis approach to hybrid materials whereby inorganic semiconductor materials are employed as catalysts and structure directing agents in biopolymers building up.

Following this bioinspired synthesis strategy, TiO_2 photocatalytic activity was exploited to drive 5,6-dihydroxyindole-2-carboxylic acid (DHICA) polymerization to



activation under visible light [1-3]. This strategy led to eco-friendly melanin- TiO_2 hybrid nanostructures with unique antimicrobial activity even under visible light [2]. Mechanism underlying formation of Melanin- TiO_2 nanoparticles was outlined by integrating Photolumiscence (PL), UV-Vis, Electron Paramagnetic Resonance (EPR) and Solid-phase Nuclear Magnetic Resonance (NMR) spectroscopies [1] (Figure 1).

DHICA polymerization to eumelanin was confirmed by EPR spectrum of nanostructures, showing a single central symmetric peak at a g-factor value of 2.0035 ± 0.0004 , which is typical of carbon-centered radicals in melanin backbone.

Furthermore, a characterization by multiple techniques allowed to link physicochemical properties of these nanosystems to their relevant biocide efficacy. Actually, both organic and inorganic phases strongly affect each other during *in-situ* formation, as far as it concerns both morphology and microstructure. DHICA polymerization

onto TiO_2 changes final morphology of TiO_2 nanostructures, as shown by TEM micrographs (Figure 2).



DHICA/Eumelanin Relative Amount

Fig. 2: TEM micrographs of bare TiO₂, TiO₂-DHICA and Eumelanin nanoparticles.

Furthermore, narrower ΔB values than bare melanin, driven from EPR spectra indicate a different spatial distribution of radical species within the hybrids, suggesting that the presence of TiO₂-sol modulates the melanin macromolecule organization, allowing an enhanced antimicrobial activity (Figure 3).



Antimicrobial activity

Fig. 3: Antimicrobial activity of TiO₂, DHICA-melanin and hybrid TiO₂-DHICA nanoparticles.

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1B – Protein trapping within nanostructured surface

G.M.L. Messina, G. Marletta

Aims

The development of a new technique enabling the fabrication of large area patterns of polymeric nanowell arrays on flat metallic surfaces, with high yield, controllable thickness, and high uniformity over large areas is described.

In particular, the proposed methodology can provide both homogenous or hybrid nanowells, providing an optimal solution to the problem of how to easily construct biosurfaces that are able to communicate with biological systems in the 'correct' way, allowing selective trapping of specific biomolecules as well as influencing their partial or complete orientation and unfolding, and finally affecting their biofunctionality.

Results

Nanostructured surfaces have generated great interest because their size, shape and local composition properties, being compatible with those of biological molecules and systems, promise in principle the manipulation of biological processes at subcellular level.

The build-up of nanostructured surfaces has been obtained by means of a large number of top-down methodologies, like photo-, electron- and ion-beam lithography, producing structures with dimensions far below 100 nm. However, these methods have the considerable drawback of involving serial and cost-consuming processes, suitable only for small area treatments.



Fig. 1: Schematic representation of the procedure applied for the preparation of the nanocavity array (PMMA on Au).

Alternatively, recent research has identified the use of self-assembly processes, operating in a parallel way, as the most promising way to achieve surface nano-structuring for large areas.

These methods, globally referred to as colloidal lithography, have shown great potential to significantly improve the performance of biosurfaces.

We describe a simple and versatile method to obtain large-scale arrays of hybrid polymer/gold nanowells, able to selectively trap different types of molecules, including drugs and proteins. The appropriate choice of materials and process

conditions, such as the colloidal nanoparticle size and the post-deposition treatments (i.e., the UV-ozone), allows the volume of each nanowell to be turned and, in turn, the overall trapping capability of arrays of nanowells of given size. This implies the possibility of further developing bioactive surfaces, i.e., surfaces able to modulate the local concentration of bioactive molecules, capable of interacting with the nanometric features of cells.



Fig. 2: AFM height images and corresponding section analysis for: (A) bare nanowell arrays, (B) nanowell arrays exposed to HSA, (C) nanowell arrays exposed to Lyz, (D) AbB HSA on HSAB containing nanowell arrays and (E) AbBLyz on nanowell exposed to Lyz.

It should be further stressed that, besides the practical interest of having bioactive surfaces, the reported results open up a wide and still little explored field of study, regarding new nanoconfinement-related properties.

Indeed, the observed counterintuitive trapping of a large protein, such as HSA, versus the untrapping of a smaller protein, like Lyz, must be considered a peculiar feature due to nanoconfinement. The proposed explanations for the phenomenon range from the nanoconfinement-induced decrease in the out-diffusion coefficient of large trapped biomolecules, to the preferential sticking of unfolded single protein molecules, to the modulation of conformational rearrangement due to the soft-hard nature of the different proteins. In fact, much more experimental and theoretical work is needed to propose a satisfactory model relating the nanoconfinement constraints to the peculiar protein behaviour. Thus, for instance, the study of the behaviour of proteins featuring similar size and overall charge could shed light on the dependence of the trapping selectivity effect on the protein softness/hardness. According to the above, we suggest that the reported results may pave the way for the construction of a new generation of bioactive surfaces, able to perform a range of actions, from filters discriminating hard–soft proteins, to more general conformationally modified biomolecules, to local providers of biosignalling molecules.

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1B – Role of polymer molecular weight on the removal process using amphiphilic formulations

M. Raudino, G. Selvolini, P. Baglioni

Aims

Study of the interaction between a non-ionic surfactant ternary system and a thick polymer film. Effect of polymer molecular weight on the rate and the efficacy of polymer dissolution.

Results

Polymer dissolution plays a key role in a wide variety of practical applications, from industrial processes to biomedical applications and, recently, in conservation science for the removal of hydrophobic polymeric films used as consolidants. Amphiphilic formulations (micellar solutions or o/w microemulsions) are usually use as efficient cleaning media but the comprehension of the main parameters affecting the mechanism of polymer removal is still limited because of the complexity of the process.

We investigate for the first time the overall interaction process between a thick polymeric film and a water/2-butanone/non-ionic surfactant ternary system by combining different techniques, mainly confocal microscopy. Our results indicate that the cooperation between the surfactant and the organic solvent is necessary to ensure good cleaning performances to the formulation. Furthermore, this experimental approach allows to clarify different aspects of the cleaning process, such as the role of polymer molecular weight on the mechanism and the kinetics of the process.

Confocal scans acquired on polyvinyl acetates with molecular weight ranging from 75 to 855 kDa incubated with the cleaning fluid reveal that the interaction mechanism between the polymer and the liquid phase strictly depends on the molecular weight and the chain entanglement of the polymeric network: low M_w systems undergo polymer removal, while for higher M_w polymers only a partial swelling of the film occurs.



Fig. 1: Confocal horizontal scans obtained on low M_w (left) and high M_w (right) polyvinyl acetate films (red) incubated with water/nonionic surfactant/2-butanone ternary system (green).

By analysing several confocal images of the film acquired at different incubation times with the liquid phase, we have seen that the removal efficacy strongly depends on the chain entanglement: the higher the M_w and so the entanglement of the polymeric network is, the lower is the efficacy of the cleaning medium in the detachment of the polymer from the substrate. In addition, we have observed that polymer polydispersity plays a key role in the overall removal process since it strongly affects the removal rate. In fact, polydisperse systems (in our case high M_w polymers) show a faster dissolution rate with respect to less disperse polymers probably due to an enhancement of the velocity of solvent penetration inside the polymeric network through defects.

Our results are in good agreement with the findings of literature on simple systems consisting of polymeric films in contact with good solvents and this is the first time that the influence of both M_w and polydispersity on the removal process of polymeric films is studied using complex amphiphilic formulations as cleaning media instead of neat organic solvents. Moreover, we have demonstrated that the new experimental method based on the use of confocal microscopy developed in this work can be a valuable approach to clarify the process of cleaning also in the case of complex systems.

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1B – Structure-property relation in oil soluble dispersants for lubricant media

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Aims

Colloidal behavior of nonionic surfactant in mineral oil. Microstructure and composition of carbonaceous deposits in lubricant media.

Results

The main objective of this work is to develop a model to connect the structural properties of dispersant additives with their efficacy against the agglomeration of carbonaceous particulates in lubricant formulations. Usually, dispersant performances are evaluated by means of expensive and time-consuming engine tests; for this reason, the research of new lab-scale methodologies to evaluate the performances of a lubricant formulation is compulsory. To accomplish this goal, we optimized different methodologies to study both the colloidal properties of the additives and their dispersant efficacy in model systems that mimic a lubricant oil. The final goal is to establish a structure-properties relation and concurrently understand the main factors affecting the dispersant ability of an additive.

The first step of the work is the identification of a carbonaceous particulate, mainly carbon blacks, to use as a model substrate. We have separated a soot-in-oil particulate and characterized it in terms of composition (elemental analysis and infrared spectroscopy), morphology (scanning electron microscopy) and fractal dimension (small angle X-ray scattering) against commercially available carbon blacks. We



found that this particulate has globular primary units with diameter ranging from 5 to 80 nm, which cluster to form aggregates.

From a compositional point of view, the particulate is mostly composed of carbon. Other elements, such as hydrogen and oxygen, are usually present in small quantities and tend to concentrate on the surface of the particle. Comparing the properties of the isolated soot with those

of different commercial particulates, Vulcan XC72 was chosen as the model substrate. The second step of the work is the study of the properties of a minimal lubricant formulation (base oil + dispersants): adsorption isotherms and optical microscopy were employed to evaluate the interaction between different dispersants and the carbonaceous substrate. In particular, we have studied a series of dispersants with different length of polar head and different number of alkyl chains. Our results indicate that, depending on the chemical nature of the amphiphile, the adsorption follows a mono-Langmuir or a di-Langmuir mechanism and the strength of the

interaction increases with the surface area of the polar head. Moreover, from optical dispersion tests, the main evidences are that mono-dispersants are less efficient than bis-dispersants and their performances are strictly connected to the dimension of the polar portion. From small angle X-ray scattering measurements, we have found that all amphiphiles form inverse cylindrical micelles in oil with dimensions depending on



the volume of the polar fraction of the dispersant.

The aggregation number for mono-dispersants is higher if compared to bis-dispersants: this is

an evidence of the higher solubility of bis-surfactants in oil, driving their higher efficacy as compared to mono-structures.

The same kind of approach was repeated in the case of complex formulations (oil + dispersants + other additives) with the aim to understand if and how the presence of other additives influences the efficacy of the dispersants. From dispersions tests we have shown that, increasing the complexity of the formulation, the dispersant efficacy decreases significantly, especially in presence of detergents and antiwear agents. This is a clear confirmation that the interaction between the dispersants and the other additives inside the lubricant formulation causes a depletion of the active dispersant fraction in the oil.

The results of this study represent an advancement in the knowledge of lubricant chemistry



and in the comprehension of the main parameters affecting the dispersant performances of different kinds of amphiphilic molecules. The simple developed labscale methodologies can be surely useful to rank different structures of dispersants in simple and complex lubricant oils to screen these formulations before expensive motor tests. Moreover, the correlation between the colloidal behavior of the amphiphiles and their dispersant efficacy can be used to guide the synthesis of novel oil soluble dispersants with enhanced activity against the carbonaceous particulate deposition in lubricant media.

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1B – Relation between structural and diffusional properties in classical and semi-IPN hydrogels

M. Rossi, G. Ferraro, E. Fratini, P. Baglioni

Aims

Synthesis and characterization of pHEMA classical and semi-interpenetrating with poly acrylic acid hydrogels. Diffusion processes of molecules and macromolecules in gels.

Results

We synthesized and characterized classic poly HEMA and semi-interpenetrating poly HEMA/PAA hydrogels having different cross-linker/monomer ratio. These differences affect the network structure and the diffusional properties of the hydrogels. Considering poly HEMA hydrogels, an increase of cross-linker percentage doesn't significantly change the nanoscale structure of the polymeric network while decreasing the free/bound water ratio (Cfree/Cbound) (left figure) and the diffusion coefficient of the molecular probe, fluorescein isothiocyanate (FITC). A sigmoidal trend of the diffusion coefficient vs Cfree/Cbound (right figure) indicates that the diffusion becomes completely activated only when the hydrogel reaches a water-percolated state.



Two series of semi-IPN poly HEMA/PAA were synthesized, one with the same ratio 8:1 between HEMA hydroxyl groups and PAA carboxylic groups and different water content (38%, 50%, 60%), the other with a water content of 38%, but different HEMA/PAA ratio (i.e. 8:1, 4:1, 2:1). SAXS analysis reveals the existence of solid-like inhomogeneity and, in the case of HEMA/PAA 8:1 series, FITC and FITC dextran 4 kDa can enter all these three hydrogels, while FITC-dextran 40 kDa can penetrate only the network with 60% H_2O . In the case of poly HEMA/PAA 4:1 and poly HEMA/PAA 2:1, it was possible to establish that FITC, FITC-dextran 4 kDa and FITC-dextran 40 kDa can diffuse into both networks. The diffusion coefficients increase with the water content and with the decrease of the amount of PAA, as the result of a lower interaction between the probes and the polymeric network.

All the results taken together provide a complete picture of the relationship between the structure, water state and diffusional properties in poly HEMA classical and semi-IPN hydrogels.

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1B – Biomimetic membranes and interaction with nanosystems

C. Montis, D. Berti, P. Bergese

Aims

Build-up reliable biomimetic membranes, capable to mimic both eukaryotic and prokaryotic cell membranes, to investigate their interaction with exogenous species, particularly nanosystems of interest for biomedical applications.

Results

Nanosystems have highly promising applications in Nanomedicine. A key issue, limiting their translation into effective application, is that the understanding of their fate in biological media and of their interaction with biological interfaces is still lacking. In this respect, artificial, biomimetic membranes have been developed. They permit working with simplified systems, and are good models to decompose the elementary events (biochemical, physical, and chemical) at stake in real biological situations.



We built-up different membrane models, of different architecture and curvature (liposomes, Giant Unilamellar Vesicles, Supported Lipid Bilayers) mimicking selected features of interest of eukaryotic and prokaryotic cells. The physicochemical characteristics of the membranes were determined in terms of morphology, structure, fluidity and through permeability Scattering methodologies (Dynamic Light Scattering, Small-angle X-ray Scattering), Steady state Fluorescence, Confocal

Microscopy, Fluorescence Correlation Spectroscopy. Their interaction with exogenous species was then investigated with the same techniques, in particular: the effects of gold nanoparticles of different surface functionalization on Giant Unilamellar Vesicles; the reconstitution of membrane proteins in lipid membranes, the interaction of a nanostructured antimicrobial system with synthetic lipid membranes mimicking relevant features of prokaryotic cells.

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1B – Lipid-SPIONs mixed assemblies as smart drug delivery systems

A. Salvatore, C. Montis, M. Mendozza, B. Castroflorio, D. Berti, P. Baglioni

Aims

Build-up smart drug delivery systems of lipid architectures with Superparamagnetic Iron Oxide Nanoparticles (SPIONs) embedded, responsive to different static and alternating magnetic fields in a tunable manner.

Results

The design of nanostructured drug delivery systems (DDS) that improve the efficacy of therapeutic principles by enhancing their biocompatibility, bioavailability and targeting, has been the focus of extensive research over the past years. Of particular relevance in this field is the development of multifunctional architecture that can deliver different therapeutic or diagnostic agents and release them in a controlled way.



In this context we designed, prepare and characterize DDS where hydrophilic and hydrophobic superparamagnetic iron oxide nanoparticles (SPIONs) are included in pure lipid and lipid-DNA mixed architectures to build-up multifunctional drug delivery systems, able to release their payload in a controlled way, through the application of low-frequency alternating magnetic fields of defined frequencies.

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1B – Poly(ethylene glycol)-*graft*-poly(vinyl acetate) single-chain nanoparticles for the encapsulation of small molecules

A. Bartolini, P. Tempesti, C. Resta, D. Berti, P. Baglioni

Aims

Synthesis and Characterization of single chain nanoparticles (SCNPs) of poly(ethylene glycol)-*graft*-poly(vinyl acetate). Use of the so-obtained single-chain globular particles to encapsulate small hydrophobic molecules therefore promoting solubilization of flavors or drugs, which could be of interest in the food and pharmaceutical industry.

Results

This work focused on the preparation of SCNPs composed of a poly(ethylene glycol)graft-poly(vinyl acetate) (PEG-g-PVAc) amphiphilic copolymer, with a very low degree of grafting. This peculiar chemical structure allows for the folding of PEG over the PVAc side chains, triggering the formation of single-chain globular objects driven by hydrophobic interactions. Both light and X-ray scattering experiments show that at 25 °C aggregation is negligible even at concentrations up to 10% w/w. When in the folded state, the hydrophobic core of these SCNPs acts as a storage compartment for small hydrophobic molecules of interest, *e.g.* flavors or drugs.

First of all, we studied the behaviour of PEG-g-PVAc aqueous solutions at different concentrations.



Fig. 1: (A) Autocorrelation functions of PEG-g-PVAC at various concentrations in water measured at 90°: Inset shows the diffusion coefficients obtained at different concentrations. (B) AFM image of PEG-g-PVAc SCNPs (scale bar is 200 nm, inset bar is 100 nm). (C) AFM line profile of two PEG-g-PVAc SCNPs highlighted in the inset of B (red ellipse). (D) SAXS data for sample AP1 together with the fit (black solid line).

DLS experiments (Fig. 1A) show the normalized autocorrelation functions at concentrations ranging from 0.1 to 10% w/w. The curves show the presence of one relaxation process and are superimposable up to 5% w/w. The hydrodynamic radii, obtained from the data analysis of the autocorrelation functions is invariant with concentration up to 5% w/w. This fact is indicative of the presence of PEG-g-PVAc SCNPs.¹

AFM measurements (Figure 1B) show the presence of spherical objects with a diameter of about 20 nm (Figure 1C). Furthermore from the SAXS curve reported in Figure 2D we calculated the molecular weight of the scattering particles using the following equation:²

$$M_{w} = I(0)N_{a}/(\Delta\rho)^{2}cv \tag{1}$$

where I(0) is the forward scattering intensity *i.e.*, the intensity at the lowest Q-values, Δq^2 is the contrast factor, N_a is Avogadro's number, *c* is the concentration in g mL⁻¹, and *v* is the polymer's specific volume in mL g⁻¹ (calculated considering a 40/60% PEG/PVAc ratio). In this way a molecular weight of 10.8 kDa is obtained, which is in very good agreement with the molecular weight of a single PEG-g-PVAc molecule. Once demonstrated the PEG-g-PVAc ability to self-fold into SCNPs, we exploited the hydrophobic nature of the core by encapsulating small molecules of interest that

possess a low solubility in water. We focused on food grade molecules such as R-(+)-Limonene, p-Anisaldehyde and A Terpinyl Acetate.

The fittings of the DLS autocorrelation functions of the flavor-loaded samples, shown in Figure 2A, result in an increase of the hydrodynamic radii of the particles up to 135%, indicative of an upload of molecules inside the core of the SCNPs.



An additional confirmation was obtained by cloud point

Fig. 2: (A) DLS profiles and (B) Temperature-Turbidity curves of samples containing 1% w/w of PEG-g-PVAc and different flavors.

determinations, since the incorporation of molecules in SCNPs leads to the modification of this critical temperature.³ From the comparison between the temperature-turbidity curves of loaded and unloaded samples (Figure 2B) we observe a decrease in the cloud point of PEG-g-PVAc SCNPs, that is a straightforward evidence of a successful encapsulation.

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1B – Delivery of nucleic acid-based therapeutics for the treatment of antibiotic-resistant pathogens

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Aims

Properties of a complex between a cationic bolaamphiphile and an oligonucleotide with antibacterial action. Delivery to antibiotic-resistant bacteria by using liposomes.

Results

This work, funded under the 7-People Framework Marie-Curie Industry and Academia Partnerships & Pathways scheme (grant agreement nr. 612338), focused on the encapsulation and delivery of Transcription Factor Decoys (TFDs): these oligonucleotides interact with essential genetic pathways in bacteria and prevent their survival response to antimicrobial attack. TFDs have proven successful in defeating infections by antibiotic-resistant bacteria *in vivo* when coupled to a cationic bolaamphiphilic molecule, 12,12'-(dodecane-1,12-diyl)-bis(9-amino-5,6,7,8-tetrahydroacridinium) or 12-bis-THA. The latter is reminiscent of Dequalinium®, an antimicrobial molecule used in commercial topic formulations, and as such possesses intrinsic antibacterial properties.

First of all, we studied the behaviour of this bolaamphiphile in aqueous solution: thanks to DLS and cryo-TEM, we found out that 12-bis-THA (chloride salt) forms bolasomes, *i.e.* vesicles, upon strong vortexing of its dilute solutions. These structures are however kinetically unstable and can be preserved only at 4 °C for a limited time,

while at room temperature they rapidly convert into onedimensional elongated assemblies (ribbons).

Next, we demonstrated, through steady-state fluorescence spectroscopy and circular dichroism (figure on the right), that the interaction between this bolaamphiphile and the oligonucleotide leads to strong binding and condensation of the TFD, which renders it resistant to nuclease digestion. We also showed that the TFD/12-bis-THA complex is reversible by



breaking it with sodium taurocholate, which competes with the TFD's polyanionic backbone for interaction with the bolaamphiphile.



designed POPC - and POPC/DOPE - based liposomes as delivery vectors to ensure colloidal stability protect the complex, and ensure its therapeutic action. DLS and Zeta- potential measurements proved that both types of liposomes were able to incorporate 12-bis-THA and possessed the appropriate size and surface charge to be used as effective DNA carriers. Both types of liposomes were loaded with a green-fluorescent TFD and challenged against a colony of E. coli which of the had membrane been labelled with а redfluorescent dye for observation with confocal laser scanning microscopy. Experiments showed that POPC-only liposomes (figure on the

left, panels a and b) interacted at the poles and septa of the bacteria, which are especially rich in a strongly anionic lipid, cardiolipin, suggesting a possible targeting mechanism for 12-bis-THA. However, only POPC/DOPE-based liposomes delivered the TFD into the bacterial cytoplasm, demonstrating the necessity of a fusogenic lipid to yield transfection.

3 µm

3 µm

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3 µm

(d)

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However, the 12-bis-THA/TFD nanoplexes presented very scarce colloidal stability in saline solutions at physiologic ionic strength and in common buffers. We therefore

1B – Complexation of short ds RNA/DNA oligonucleotides with Gemini micelles: a time resolved SAXS and computational study

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Aims

One major challenges in gene therapy is the development of non-viral vectors for genetic material, such as plasmids and small interfering nucleic acids. The molecular properties of complexes between carriers and nucleic acids are of fundamental importance to obtain efficient transfection. In this contribution we describe the structural evolution of oligonucleotide (siRNA or siDNA) during complexation with micelles of divalent cationic surfactants, i.e. Gemini bis (quaternary ammonium) bromide with variable spacer length (12-3-12, 12-6-12, 12-12-12).

Results

The kinetics of complexation was studied by time resolved Small Angle X Ray Scattering (SAXS) performed at the European Synchrotron Radiation Facility (Grenoble, France) and by molecular dynamics. In SAXS experiments all the systems contained a fixed amount of surfactant and different concentrations of oligonucleotide at charge ratios (+/-) 0.75 and 1.25. SAXS intensity diagrams showed that complexes appear in solution immediately after mixing (10-20 ms) and, therefore, the study of their formation requires fast experimental techniques. The obtained aggregates have internal arrangement constituted by layers of squeezed micelles alternating the nucleic acids. Moreover, we found that there are relevant differences in the structure of the nucleic acid/micelles complexes due to the nature of the nucleic acid (siRNA and siDNA). To illustrate this point figure 1 shows the comparison of SAXS profiles obtained for siRNA and siDNA complexed with 12-6-12 micelles.



Fig. 1: SAXS diagrams of siRNA/12-6-12 and siDNA/12-6-12 (20 ms after mixing).

Molecular dynamics simulations were carried out to obtain an atomistic description of the interaction between the nucleic acid molecules and the surfactant aggregates. The systems composed by siDNA or siRNA, 27 molecules of Gemini 12-6-12 (CR = 0.75), ~15000 water molecules and ions (40 Na+ and 54 Br-) were simulated for 100 ns (after 20 ns of equilibration) at P = 1 bar and T = 298 K. The corresponding snapshots are reported in figure 2.



Fig. 2: Snapshots of the siRNA/12-6-12 (right) and siDNA/12-6-12 (left) complex at the starting point and after 100ns of MD simulation.

The analysis of MD trajectories put into evidence a preferential interaction of the micellar aggregates with the minor groove of the nucleic acid. The siRNA associated with the micelles conserve a more compact structure (\sim 1.9nm) respect to the siDNA (\sim 2.2nm). Moreover, the siDNA associated to the micellar aggregates presents a greater deformation respect to siRNA, as evidenced by the root mean square deviation, calculated respect to initial structure of siDNA and siRNA, that reaches the value of 0.80 and 0.51 nm respectively.

These results are in agreement with those obtained by SAXS and provide refined information on the structure of complexes formed by Gemini micelles and siRNA or siDNA oligonucleotides.

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1B – Nitric oxide assisted C60-SIMS for molecular depth profiling of polyelectrolyte multilayers

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Aims

Molecular depth profiling of polymers is an important demand in many technological applications that has been increasingly fulfilled by the introduction and development of cluster SIMS methodologies. SIMS with polyatomic primary ions provides a successful tool for molecular depth profiling of polymer systems, relevant in many technological applications. Widespread C_{60} sources, however, cause in some polymers extensive damage with loss of molecular information along depth. We studied a method, based on the use of a radical scavenger, for inhibiting ion beam-induced reactions causing sample damage.

Results

The introduction of reactive gases during SIMS analysis turned out to be an interesting aid in organic and polymer depth profiling, either for obtaining an increase of ionization efficiency [1] or for interfering with adverse ion beam-induced reaction (such as crosslinking) that in some cases prevent the accomplishment of a successful molecular depth profile. The latter approach, initially proposed by our laboratory, consists in the use of a radical scavenger, namely nitric oxide (NO), and it has been recently shown to be a valid and cheap tool, in alternative to the more effective GCIBs, for extending the use of fullerene beams in depth profiling of difficult polymers [2]. Moreover NO flooding in conjunction with fullerene primary beams allows the analysis of hybrid organic-inorganic systems [5] and, in addition, it can supply some additional indication useful for a deeper understanding of the ion-beam induced chemistry in polymers.

We present some recent results obtained on multilayers with NO-assisted C_{60} -SIMS depth profiling. In particular we prepared and examined some test samples based on layer-by-layer (LbL) deposition of polyelectrolytes, which is a versatile technique that allows to cover any kind of surfaces with well-ordered films by fine tuning of thickness and composition. In particular, we used polydiallyldimethylammonium chloride (PDDA), poly acrylic acid (PAA) and polystyrene sulfonate (PSS) as polyelectrolites and combined them in order to obtain multilayers with different sequences of the three components.

Such layers where profiled by C_{60} -SIMS and the influence of NO and sample temperature in terms of damage accumulation, erosion yield and depth resolution was investigated.[3].

As shown in Figure, C_{60} depth profiling in standard conditions (i.e. without NOdosing and at RT) does not allow to obtain satisfactory molecular depth profiles when relatively thick PSS-based layers are involved, due to ion-beam-induced crosslinking occurring in this system. By contrast, the introduction of NO allows to obtain in all cases good molecular depth profiles and to discriminate, on the basis of the intensity of structure-related fragments, among all the layers, with satisfactory depth resolution and sputter yield. A further improvement in the quality of the profiles can be obtained by cooling the sample down to 150 K. Actually it has been already reported that

temperature affects[4] the quality of depth profiles of polymers, and this is not surprising if we consider that chemical reactions are involved in the erosion process.



Fluence (1015 ions/cm2)

The above findings confirm the ability of nitric oxide to inhibit radical reactions leading to cross-linking and damage accumulation during C_{60} SIMS depth profiling of polymers and prompt NO-dosing method as a valuable one for the SIMS characterization of polymer multilayers with C_{60} primary beams. Although similar and even better results have been recently obtained by means of large polyatomic argon clusters (GCIB), NO-dosing has the advantage of allowing to continue to use the widespread C_{60} sources and, moreover, it is expected to be useful when profiling hybrid organic/inorganic multilayers. Indeed GCIBs are not able to profile inorganic materials at the low energies per constituent atom that are suitable for organic molecular depth depth profiling, while a fullerene beam with the aid of NO-dosing should be suitable for this purpose.

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1C – Active sites of copper-trafficking proteins: density functional structural and spectroscopy studies on copper(I) models

C. Rossi, G. Tamasi, C. Bonechi, A. Donati, A. Magnani

Aims

Several proteins are believed to be actively involved in copper trafficking and storage, and even small biomolecules such as glutathione (GSH) play an important role in binding copper *in vivo*, and sometimes copper proteins are involved in serious human diseases like Parkinson and Menkes pathologies. Structural studies at metal sites might help in understanding the molecular mechanism of such health disorders. In the present work, selected structures optimized via density functional (DFT) methods of some models of copper(I) binary and ternary complexes, with low-molecular weight ligands, on the relevant selected computed structural parameters, spectroscopic data, and energy aspects, are reported. These data can help in interpreting structural data of complex biological systems and in constructing reliable force fields for molecular mechanics computations.

Results

The work provided rationale for several structural features of selected copper protein systems involved in copper trafficking found experimentally at the solid state and in the solution phase via X-ray diffraction and NMR techniques, especially those that involve mononuclear coordination.

A series of mononuclear binary and ternary Cu(I) complexes with formato, formamide, methylphenol, and methanethiolato ligands were optimized at DFT-B3LYP/6-31G** and DFT-B3LYP/6-311++G** levels of theory. The solvent effect was taken into account via PCM method.

The investigation of estimated qualitative energy of formation of the computed models explained that the linear $Cu(I)S_2$ coordination mode was the most favorable both for thiolato (RS–) and thiol (RSH) ligands when compared to Cu(I)S, $Cu(I)S_3$ and $Cu(I)S_4$ modes. Then, the grafting on the $Cu(I)S_2$ skeleton by certain hard donor groups like alcohol/phenol(ROH) and carboxylate and amide functions are suitable for further stabilizing the overall coordination scaffolding. The treatment of solvation effects via PCM methods (solvent, water) has been also considered, showing that it did not have dramatic influence on structural parameters and on reaction energies.

The formation energies of $[Cu(HSCH_3/SCH_3)(OOCH)]^{0/-1}$ were higher than those of $[Cu(HSCH_3/SCH_3)_2]^{+/-}$ on starting from $[Cu(HSCH_3/Cu(SCH_3)]^{+/0}$ by *ca*. 10 kcal mol⁻¹ (DFT-PCM-B3LYP/6-311++G** levels of theory). The structural arrangements, bond distances, and angles as well as computed spectroscopic parameters resulted in good agreement with experimental data for corresponding to synthetic complexes and with metal site regions of several copper(I)-proteins.



Fig. 1: Cu(I)-complex models for copper trafficking protein structures.

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1C – Biopolymers and Biomacromolecules Solvent

C. Rossi, C. Bonechi, A. Foletti, G. Tamasi, A. Donati, A. Magnani

Aims

In this paper we developed a strategy, based on Nuclear Magnetic Resonance Spectroscopy, to define the dynamical contribution of the biomacromolecules to the water molecules belonging to their hydration shells.

Results

Biomacromolecules in solution modify the structure and the dynamics of the bulk water at the solute-solvent interface. The ordering effects of biomolecules, in particular proteins, are extended for several angstroms. The role of the hydration shells around a protein has yet to be completely understood. Hydrated proteins maintain more dynamic flexibility with respect to the dried system, which is an important property in protein-protein and/or protein-ligand recognition processes.



Fig. 1: Effect of the ordering effect of proteins on water. Three water environments defined by their dynamical properties can be observed: bulk, surface and buried water environments

We propose a method for analyzing the dynamical properties of the water molecules present in the hydration shells of proteins. The approach is based on analysis of the effects of protein-solvent interactions on water protons

NMR relaxation parameters. The water proton spin-lattice relaxation rate in protein solution is analyzed considering all possible dipolar contributions from coupled protons environments. The analysis of both selective and non-selective water spin-

lattice relaxation rates allowed the calculation of the average effective correlation time for the water molecules at the protein interface and the evaluation of the long range ordering effect of the protein surface.

In diluted protein solutions, the bulk water proton relaxation shared the contributions from the water molecules in the protein hydration shell. These water molecules differ from the bulk water, mainly because of their correlation times, which is are short for bulk water and longer for the protein hydration waters.

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1C - In silico design of Dyes for DSSC

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Aims

Computational chemistry methods are applied for the calculation of the electronic and molecular properties of designed compounds to be used as dyes for DSSC (Dye Sensitized Solar Cells). The main goal is to verify, even prior to the laboratory synthesis, whether: i) the semiconductor/dye/redox mediator system has a good "alignment" between the energy levels and the relevant electrochemical potentials and ii) the sensitizer has an energy gap wide enough to exploit a large portion of the solar spectrum. The computational study also allows for the characterization of the photostability of these compounds since, to be of practical interest, they must be stable in operation conditions.

Results

Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) have been used for the simulations, either in gas phase or in solution, of the absorption properties of dye molecules, mainly based on a D- π -A structure (i.e., featuring a π conjugated backbone connecting donor and acceptor/anchoring groups), providing very accurate results. Furthermore, as a first step toward the exploration of the excited state potential energy surface of the dyes and, therefore, the evaluation of the photostability, the excited state geometries and emission maxima of several organic dyes used as sensitizers in DSSCs (see molecules I–XI) have been computed and compared to the available experimental data using TD-DFT and a polarizable continuum model (PCM), both in the Linear-Response (LR) and in the State-Specific (SS) formalisms, to take into account solvent effects.



The results showed that the use of six different functionals (LC- ω PBE, LC-BLYP, CAM-B3LYP, ω B97X-D, M06-HF, MPW1K) within the PCM/TD-DFT method allowed for the accurate calculation of the low-lying singlet excited state of the D- π -A dyes obtaining emission data that compare well with the experimental values. Indeed, the mean absolute error (MAE) is, in the best cases, 0.10 eV. The inclusion of solvent effects at the optimization stage is crucial to obtain results that are consistent with experimental values (ca. 0.2 eV). The use of a SS-PCM model further reduces the discrepancy with experiments (within 0.15 eV).



To the best of our knowledge, this is (i) the first extensive TD-DFT computational study that focuses on the emitting properties of D- π -A dyes in which the role of the solvation in affecting the excited state geometries has been explored and (ii) the first computational investigation of excited state geometry and emission properties of one of the most representative organic dyes for DSSC, i.e., the D5 dye (molecule I).

The present benchmarking study opens the way to the evaluation of the photostability of D- π -A sensitizers and thus to the design of more robust organic dyes, in terms of excited state stability, through substitutions and/or insertion of different molecular units.

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1C– Computational spectroscopy of protein radicals

C. Bernini, R. Basosi, A. Sinicropi

Aims

State-of-the-art quantum-mechanics/molecular-mechanics (QM/MM) methods are used to characterize the electronic, vibrational, and magnetic properties of redoxactive amino acids involved in long-range electron transfer pathways in proteins. The results obtained are expected to shed new light on the catalytic mechanism involving radical species and thus open the way to a comprehensive understanding of radical-mediated ET reactions.

Results

Hybrid QM/MM methods, in combination with methods of molecular dynamics (MD), have been used to characterize protein radicals, mainly tryptophan and tyrosine radicals, involved in long-range electron transfer pathways of several proteins/enzymes. In particular, we employed density functional theory and multiconfigurational perturbation methods to construct QM/MM models of i) versatile peroxidase (VP) from *Pleurotus eryngii* and its W164Y variant; ii) lignin peroxidase (LiP) from Phanerochaete chrysosporium, two engineered variants of LiP and Coprinus cinereus peroxidase (CiP); iii) two Pseudomonas aeruginosa azurin mutants (Az48W and ReAz108W). The models have been capable of reproducing specific features of their observed UV-Vis, resonance Raman, and electron paramagnetic resonance spectra. The proper modeling of the environmental effects within the QM/MM protocol, in combination with the available experimental data, has made it possible the unambiguous assignment of the experimentally detected radical species and the clarification of the nature (neutral deprotonated or cationic protonated) of the intermediates. Furthermore, it allows to obtain a mechanistic description of the proton-coupled electron transfer process leading to the radical formation and to provide additional details on the role played by the nearby protein residues and

solvent water molecules in affecting the spectral properties and the geometrical structure of the radical intermediates.

More recently, we built models of tryptophan and tyrosine radicals within the protein matrix of the cytochrome c peroxidase (CcP) from *Saccharomyces cerevisiae*. Cytochrome c peroxidase (CcP) is a heme-containing enzyme involved in the mitochondria electron transport chain. Similar to other heme peroxidases, the ferric resting form of CcP is first



oxidized by H2O2 to a two-electron oxidized intermediate (Cp-I), in which one oxidizing equivalent is stored as an oxoferryl species, while the second one as a protein radical. Cp-I is then reduced by two molecules of Cytochrome c to cycle back

to the resting enzyme. Electron paramagnetic resonance (EPR) and electronic and nuclear double resonance (ENDOR) measurements indicated that both a tryptophan and a tyrosine radical contributed to Cp-I. Despite this, no definitive answer on the assignment of the radical species to a specific tryptophan and tyrosine residue has yet been provided. Moreover, so far, the neutral or charged nature of the tryptophan radical has not been clearly indicated. The results show that the models correctly predict the magnetic, electronic and vibrational properties of the observed amino acid radicals of Cp-I and demonstrate that a tryptophan cationic radical (Trp191•+) and three tyrosine residues (Tyr203, Tyr236 and Tyr251), located along two possible ET pathways involving Trp191•+, are possible candidates to host the Cp-I radical species.

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1C- A complex system's view of the rebound effect in energy efficiency

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Aims

The project aims to provide a characterization of the rebound effect by means of complex systems methods (nonlinear systems dynamic and complex networks).

Results

There is evidence that energy efficiency improvements do not ultimately produce the expected results in terms of energy savings. This phenomenon is due to the so called *rebound effect*. Indeed, for households and firms an energy efficiency improvement is equivalent to a reduction of the cost of the energy service that has been improved, that is, they can obtain the same amount of useful work from the improved energy service (e.g. thermal comfort, travelled kilometers, lighting, etc.) at less cost (or alternatively, more useful work at the same cost), which would lead to a subsequent increase in the energy consumption, offsetting partially or completely the energy savings derived from the energy efficiency improvement.

Even when maintaining the same useful work at the same cost, an energy efficiency improvement produces qualitative changes in energy service in the form of improving attributes or characteristics, therefore resulting in an alternative form of rebound effect. Regarding this, there is a general agreement between energy economists about the existence of rebound effect. Disagreement however centers on the sources and especially from the size it achieves. Some authors claim that it is less than 100%, that is, the energy efficiency improvements produce a net reduction of energy consumption. Alternatively some of them argue that it is higher than 100% and therefore energy efficiency improvements lead to a "backfire", producing an increase in the final energy consumption.

Understanding this distinction involves an effort and the need of a paradigm shift when dealing with the rebound effect.

In the present project, we make the assumption that the rebound effect is the result of a set of nonlinear interaction producing an emergent behavior that can be modeled by means of the methods typical of complex systems sciences. Our starting point is the consideration that evolutionary systems, such as biological or even socio-economic systems, may evolve towards more complex structure under the pressure of an increasing flow of energy and materials, driven by the higher conversion rate of greater efficiency. Higher complexity, due to a greater energy density rate, counteracts the positive effects of energy efficiency, resulting in a increase of resource consumption.

More specifically, our aim is to apply the methods of complex networks and systems dynamics to model, explain, and quantify the rebound effect in the energy systems, with an application to urban ecosystems and transport infrastructures (also including the effect of rebound dynamics in a scenario of wide diffusion of electric mobility). We use the above mentioned methods because:

1) **Complex networks** are a well established paradigm for modeling and describing different systems interconnected both in a physical and functional way. This characteristics makes them suitable to model the connection of urban infrastructures, that as the city evolved become more an more interconnected, as showed in figure 1.

2) **Nonlinear Systems dynamics** is the appropriate framework to describe the temporal evolution of systems with nonlinear feedbacks that, due to bifurcations and changes in their stability characteristics can be useful in modeling the rebound dynamics.



Fig. 1 Interdependence of urban infrastructures

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1C - Leather production ultrasound-assisted as best available technology to reduce damages to workers health

G Bufalo, F. Di Nezza, L. Cimmino, F. Cuomo, L. Ambrosone

Aims

One of the purposes of this paper is to show how applying ultrasound to tanning-alumwater greasing approach to produce mink fur with desired quality.

Results

The environmental impact of fur industry is quite relevant. Measurements carried out on mink fur show that ultrasound have a limited effect on the diffusion rate, but increase the capacity of the tanning-greasing agent only after attainment of the equilibrium. Experimental results indicate that cavitation greatly improves the greasing-tanning stage increasing the skin absorption of 25%. This implies a reduction of volatile solvents load of 50%. Since the mink fur is machined in open standing

paddle, such reduction significantly increases the working place healthiness. Experimental results can be transposed to industrial scale in two possible arrangements. However, the configuration with all transducers outside of the reactor appears to be more suitable for the mink fur production. This is because with standing paddle open and fixed one is able to irradiate a welldefined area, increasing the quality of the final fur. In this way, the equipment costs are lowered, the environmental impact is reduced, the



toxicity of the volatile solvents partially torn down and finally the product quality is optimized.

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1C – Specific Ion Effects in Protein Systems

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Aims

Investigation of specific ion effects in protein systems. The specific effect of cations suggests that they operate through two opposite mechanisms. A new theoretical modelling is being developed.

Results

Specific ion effects are those variations in properties which are not anticipated from classical electrostatic theory of salt solutions. They were firstly observed in 1888 by Franz Hofmeister who studied the effect of salt addition on the aggregation of egg white proteins. He ordered the salts, with the same cation but different anions, according to their ability in promoting the precipitation (salting-out) or the solubility (salting-in) of a protein in aqueous solution. A conventional 'Hofmeister series' is: $HPO_4^{2-} > SO_4^{2-} > F^- > CI^- > Br^- > NO_3^- > CIO_4^- > SCN^-$

The 'salting-out' anions (left side of the series) are strongly hydrated, while salting-in' anions (right side) are only weakly hydrated. A similar series for cations was also observed:

 $NH_4^+ > K^+ > Na^+ > Li^+ > Mg^{2+} > Ca^{2+}$

The 'conventional' cation series has a substantial difference compared to the case of anions.⁵ Indeed, salting-out cations are weakly hydrated (NH_4^+) and salting-in cations are strongly hydrated (i.e. Li⁺ and Mg²⁺). Substantially, anions and cations behave in the opposite way. The understanding of the specific cation behaviour is very interesting because many cations (i.e. Na⁺, K⁺, Mg²⁺, Ca²⁺) play a crucial role in fundamental biological systems. We investigated the specific effect of salts on the molecular motion of a concentrated solution of a model protein (bovine serum albumin, BSA) in physiological conditions. To investigate the subtle molecular



protein-electrolyte interactions the 'Brownian' diffusion coefficient, D_c , obtained through dynamic light scattering (DLS) measurements is an extremely sensitive and convenient

parameter. The diffusion coefficients increase according to the typical Hofmeister sequence for anions (SCN⁻ > I⁻ > Br⁻ > Cl⁻ > F⁻), usually observed for pH > pI. The observed trend is consistent with a specific anion adsorption on BSA surface, despite its negative net charge at pH 7. The higher negative charge induced by SCN⁻ adsorption at BSA surface strengthens the repulsion among protein molecules and, hence, higher D_c values are measured. The effect of different cations was then studied by measuring D_c values for BSA solutions (40 mg/mL) at pH 7 in the presence of



different 0.1 M chloride salts. Differently from the anions case, here the D_c values do not follow a monotonic series but, rather, a "bell-shaped" trend: Rb⁺ ~ K⁺ > Na⁺ > Cs⁺ ~ Li⁺. Cesium and lithium, two cations that are considered to be at the opposite sides of the Hofmeister series, behave very similarly giving rise to the lowest values of D_c . Rubidium and potassium, instead, increase BSA motion, while sodium is

in between the two extremes. A similar "bell-shaped" series for cations is a clear sign of two different mechanisms that operate in opposite directions. In the early attempts to include dispersion forces the dispersion energy, $U_{dispersion}$, was estimated from ion static polarizabilities. Since polarizability increases going from Li⁺ to Cs⁺, a stronger adsorption for Cs⁺ rather than Li⁺ at a protein surface is expected. But if we consider Collins' "law of matching water affinities" (LMWA) the formation of ion pairs between a cation and a negatively charged kosmotropic carboxylate would follow the order $Li^+ > Na^+ > K^+ > Rb^+ > Cs^+$. That is, the two approaches would predict exactly the opposite sequences. Our experimental results clearly show that both mechanism are at work and the observed macroscopic phenomenon, i.e. Brownian motion is due to a delicate interplay of these two microscopic mechanisms. On the basis of our experimental results, we are currently working to improve specific ion effects in protein systems by the theoretical point of view. The new theoretical model considers the two different hypothesized mechanisms: i. physisorption at neutral protein surface and ii. chemisorption at charged sites. Both involve, besides the conventional electrostatic forces, also polarizability-dependent ion dispersion forces.

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1C – Simulation of SIMS depth profiles of organic solids by transport diffusion model

N. Tuccitto, G. Zappalà, S. Vitale, A. Torrisi, A. Licciardello

Aims

SIMS depth profiling of organic targets is nowadays achievable thanks to the introduction of cluster beams, which allow the in-depth detection of the typical fragments of the material under investigation well beyond the so-called "static limit". Such capability depends on several physical and chemical processes following the cluster impact, which are nowadays attracting the interest of many researchers.

In this research, we develop a new model for the simulation of SIMS depth profiles, which is able to incorporate the beam-induced reactivity, so leading to a reasonable simulation of depth profiles of polymers and organic solids.

Results

During a dynamic SIMS experiment the sputter beam erodes the uppermost layers of the target reaching deeper and deeper portions of the sample with a velocity (sputtering rate) that depends on the primary beam parameters (current density, energy and type of projectile ion) and on the nature of the target. In the phenomenological model outlined here, the position of the bombarded surface is kept invariant, so that he erosion process is represented as a "travel" of the underlying material toward the surface. The sputtering rate is represented by the travel velocity, v, of the target layers travelling towards the surface. When the material moving towards the surface enters the altered layer, it is redistributed by ion-beam mixing, which can be described by a Fick-like diffusivity. [1]

If the beam does not induce reactions in the sample, the partial differential equation describing the evolution of the concentration profile C(x,t) of a certain species in the target during a sputter-profile experiment can be written as:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D\nabla c) - \nabla \cdot (\nu c) \tag{1}$$

where: C is the concentration of the species composing the target layer, v is the velocity at which the inner material is moving towards the surface (i.e. the sputtering rate), and D (corresponding to the Fick's diffusion coefficient in the diffusion laws) is a function describing the beam-induced alterations in the target. These include all the ion-beam effects leading to the formation of the altered layer (such as ballistic mixing and radiation enhanced diffusion) as well as beam-induced roughening. In the case of samples undergoing beam-induced reactions, the partial differential equation describing the evolution of the concentration C of the species of interest can be written as:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D\nabla c) - \nabla \cdot (\nu c) + R \tag{2}$$

where R incorporates all the kinetic equations of the beam-induced reactions occurring in the region involved in the sputtering process.

During a SIMS depth profile experiment on organic samples, the intensity of species characteristic of the original material is often reduced, due to beam-induced damage. A simple case that can be hypothesized is that of a single (beam-induced) reaction taking place in the sample, which produces a decrease of concentration C of the

original molecule with a first order rate law. In such instance the continuity equation that models the entire process becomes:

$$\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C) - \nabla \cdot (vC) + \left(-K_{damage} C\right) * A \tag{3}$$

where K_{damage} is the kinetic constant of the damage-producing reaction, and A is a function that takes into account the fact that the reaction is occurring in a limited depth region of the sample



We measured the SIMS depth profiles, obtained by using a C₆₀ sputter beam, of several polymers displaying different damage behavior in the same experimental conditions, namely PS, PMMA and a random PS-MMA copolymer (5% styrene-95% MMA). In Figure the experimental depth profiles (1a) are compared with those calculated by means of the transport & reaction model (1b). The simulated profiles were obtained by using the same input parameters (i.e. D, v, sample thickness) with the exception of K_{damage} , which was assumed to be 1.0, 0.05 and 0.0, for polystyrene, poly (styrene-co-MMA) and PMMA respectively. As it is evident from figure, the model is able to reproduce the essential characteristics of the experimental profiles, namely the drop of signal intensity and the decrease of the sputtering yield. This is accomplished by changing just a single parameter (K_{damage} ,) that is describing the different ion-beam induced chemical behavior of the three systems.

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1C – Automated Data Mining of Secondary Ion Mass Spectra

N. Tuccitto, G. Zappalà, S. Vitale, A. Torrisi, A. Licciardello

Aims

Secondary ion mass spectrometry (SIMS) is an important technique for the characterization of materials. However, each set of experiments produces giant raw data files composed by several spectra each containing thousands of peaks that carry the chemical information. The challenge is to perform an ease features extraction from complex polymeric and organic functional materials. We applied the wavelet transform for data compression and noise removal, followed by principal component analysis for feature extraction.

Results

Time of flight secondary ion mass spectrometry (ToF-SIMS) allows the reliable analytical determination of organic and polymeric materials. Since a typical raw data may contain thousands of peaks, the amount of information to deal with is accordingly large, so that data reduction techniques become indispensable for extracting the most significant information from the given data set. We used wavelet-PCA based signal processing of giant raw data acquired during ToF-SIMS experiments. The proposed procedure provides a straightforwardly "manageable" dataset without any binning procedure neither detailed integration. By studying the PCA results detailed and reliable information about the chemical composition of polymeric samples have been gathered.



The approach is based on the use of a "smart" data compression by discrete wavelet transform followed by PCA of the approximation coefficients and the successive wavelet inversed transformation of data. First the spectrum of each sample is compressed to the proper level of approximation by means of the appropriate wavelet function. The selection of the wavelet function and the choice of the acceptable

approximation-level are achieved by means of several quantitative estimators of the compression-quality. The wavelet-based compression procedure is able to reduce each original spectrum-data of 2^N factor, where N is an integer representing the selected approximation level. In such a way, PCA dataset matrix is assembled by using the wavelet approximation coefficients (PCA-variables) calculated at each scan (PCA-objects). Finally, Scores values of the most important Principal Components are plotted besides the reconstructed "pseudo–spectra" after the inverse-wavelet transform applied to the Loadings values. The benefits of performing the multivariate regression or classification analysis on the relevant signal part of the wavelet coefficients are reduced computation resources and time and possibly a better discrimination of most statistically important signals based of the study of the loadings from PCA.

This procedure has already been applied for the investigation of ToF-SIMS depth profiles data. [1,2] We applied such data-treatment on static ToF-SIMS spectra acquired from model polymers-based material deposited onto silicon substrate by means of spin-assembly procedure. The automated procedure allowed to obtain information about the sample, and this information is comparable to those obtained by a detailed classic single peak investigation that may have been performed by a specialist.

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2A – Environmental Assessment of total Reinjection System For Deep High Temperature/High Pressure Geothermal Resources

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Aims

The aim of the project is the life cycle analysis of technological solutions for closedloop zero emission and total reinjection pilot systems for geothermal energy production from high temperature and high pressure deep-seated sources.

Results

One of the major challenges Europe will face in the coming decades is to make its energy system clean, secure and efficient, while ensuring EU industrial leadership in low-carbon energy technologies. Geothermal energy can strongly contribute to decarbonise the energy system in a sustainable way, to secure energy supply and to complete the energy internal market in line with the objectives of the Strategic Energy Technology Plan (SET-Plan) and of the related energy legislation (notably the Renewable Energy and CCS Directives) and energy policies designed to deliver the 2020 targets and to shape energy market frameworks for 2030 and 2050. The growth of geothermal power production is mainly related to deep (> 3 km) high temperature HT (>250°C) high pressure HP (>70 bar) resources mostly located in fractured hard rock reservoirs. These resources are located in magmatic areas, which are often intensively cultivated or environmentally protected. Geothermal development in such regions can be severely hindered by the perspective of emission of Mon-Condensable Gases (NCG) in the atmosphere. Furthermore, the NCG emissions pose some concern to the effectiveness of geothermal to mitigate climate change. Lack of Social acceptability related to venting of NCG poses a major financial risk and effectively renders many prospective areas with excellent subsurface potential, which are proximal to inhabited areas in Europe, unattractive for development. Total reinjection can avoid emission of NCG, and considerable enhance resource development. However, new resource-efficient and cost-effective concepts and technologies for total reinjection are needed in order to increase the economic and environmental sustainability of geothermal projects with a minimal environmental footprint.

In this context the life cycle analysis methodology is employed in order to perform a systematic and in-depth geo-specific assessment of environmental impacts and burdens (in energy, resources and emissions terms) connected with the technological solutions used for the realization and implementation of a geothermal pilot plant with total reinjection system in the Tuscany region.

The outcomes of such analysis are pivotal to draw the eco-profile of the geothermal system in order to highlight the critical points and hot spots of the process, on one hand, and to make comparisons with other available technologies for the exploitation of the geothermal resource in similar geophysical conditions.



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2A – Biomass Adsorbent for Removal of Toxic Metal

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Aims

The contamination of water bodies by heavy metals has been the subject of many studies worldwide. Systems such as ion exchange resins, electrochemical process, chemical precipitation and activated carbon have been widely used in the processes of wastewater purification. Such processes could have reduced its costs from the use of alternative and cheaper materials. Materials of natural origin such as seaweed, biological depuration plant sludge, agricultural and industrial wastes are inexhaustible, low-cost and non-hazardous materials, which are specifically selective for different contaminants and easily disposed by incineration. Rice husk (RH) is a low cost (agricultural by-product) bio-adsorbent which has been studied intensively for the removal of various heavy metals and metalloids (such as Pb, Cd, Zn, Ni and As) from both groundwater and surface water. However, no investigations have yet been carried out about the role played by the size and shape of HR particles on the adsorption efficiency for the removal of heavy metals from aqueous solutions.

Results

A weighted amount of raw rice husk (RH), generated as agricultural waste material in a rice producing plant located in Northern Italy (Figure 1A), was washed with deionized water and let drying in ventilated oven at 40-50°C. 10 g of washed RH were grounded with a lab mill and subsequently passed through a sieve with a mesh size of 1.0 mm.

A dynamic image analyser, capable to acquire every single particle image of the sample analysed, thus ensuring a perfect statistical representation thanks to the large amount of particles (order of million particles!) analysed in a short time, was used to perform the particle size analysis of the passed RH fraction (Figure 1B).



A first indication of the high adsorption efficiency of RH toward Cd was yielded from a series of adsorption tests, where equal amounts of sieved RH (1g each sample) were left in contact with a Cd 5.4 ppm aqueous solution for increasing contact times from 1 to 240 min. Analytical determinations of residual Cd recorded vs time confirmed that

just after t = 5 min, 1 g of RH was able to adsorb 100 % of heavy metal dissolved in 100 ml aqueous solution.



Further experiments are in progress to investigate the equilibrium sorption property of RH and combine several adsorption isotherm models with physicochemical parameters of the adsorbent, such as surface area, average size and shape of particles and chemical composition.

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2A – Synergies in chemical, optical and biological conditions causing the formation of black water blooms

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Aims

Excessive production of organic matter in aquatic ecosystems can lead to a phenomena known as black water blooms. These have been associated to fish-kills and the closure of potable water supplies. The frequency and duration of these events has increased in recent decades in rivers, inland lakes and reservoirs, and has often been associated with the decay and release of organic matter (planktonic algae, aquatic macrophytes, sediment release, etc.).

Results

Using optical, chemical and biological approaches, the present series of studies shows the interactions between microbial, chemical, hydrodynamic and optical conditions necessary for black blooms to occur. The study combines field investigations and laboratory mesocosm studies to show that black blooms are caused by a combination of high CDOM (chromophoric dissolved organic matter) absorption, the formation of CDOM-Fe complexes and low backscattering. Mesocosm experiments showed that black bloom conditions occur after 4 days, with a significant increase in the concentrations of Fe2+ and Σ S2-. Total absorption (excluding absorption due to water) at 440nm increased by 30% over this time to 7.3 m-1. In addition, the relative contribution of CDOM absorption to the non-water total absorption increased from 18% to 50%. Regression analyses between chemical and bio-optical data in both field and mesocosm experiments indicated that the concentrations of Fe2+ co-varied positively with CDOM absorption ag(440) (R2 > 0.70), and the specific CDOM absorption (ag(440)/DOC). Conditions that favored the development of black blooms were elevated algal or macrophyte biomass and limited water column mixing.

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2A – Micro and macroscale drivers of nutrient pollution in freshwater environments in North and South America

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Aims

Widespread use of agricultural fertilisers has had a significant impact on freshwater ecosystems across the globe. To identify the extent of these impacts, low cost methods are combined with enagment approaches to train communities to monitor their environment for the degree of impact related to eutrophication.

Results

The present study explored the relationship of nutrient concentrations in 150 streams in 57 hydrological basins in South, Central and North America (Buenos Aires, Curitiba, São Paulo, Rio de Janeiro, Mexico City and Vancouver) with macroscale information available from global datasets and microscale data acquired by trained citizen scientists. New methods to determine average sub-basin phosphate (P-PO4) concentrations were found to be well correlated with sub-basin attributes on both macro and microscales, while the relationships between sub-basin attributes and nitrate (N-NO3) concentrations were limited. A phosphate threshold for eutrophic conditions (>0.1 mg L-1 P-PO4) was exceeded in basins where microscale point source discharge points (eg. residential, industrial, urban/road) were identified in more than 86% of stream reaches monitored by citizen scientists. The presence of bankside vegetation covaried (rho = -0.53) with lower phosphate concentrations in the ecosystems studied. Macroscale information on nutrient loading allowed for a strong separation between basins with and without eutrophic conditions. Most importantly, the combination of macroscale and microscale information acquired increased our ability to explain sub-basin variability of P-PO₄ concentrations. The identification of microscale point sources and bank vegetation conditions by citizen scientists provided important information that local authorities could use to improve their management of lower order river ecosystems.

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2A – LCA of integrated agro-industrial chains for energy and biochemicals production from micro-algae and terrestrial oilseed crops

S. Jez, E. Busi, D. Spinelli (Laboratory Manager / R&D unit, Solaris Biotechnology srl), M.L. Parisi, R. Basosi

Aims

Environmental assessment trough LCA of Integrated agro-industrial chains with high energy efficiency for the development of eco-compatible processes of energy and biochemicals production from renewable sources and for the land valorisation, within a new model of less dissipative system economy.

Results

In the framework of the EnerbioChem project (PON "Ricerca e Competitività 2007-2013") two agro-industrial (from oleaginous and lignocellulosic biomasses) and aquatic biomass (from microalgae) chains are investigated with the aim of maximizing the energetic efficiency. Valorisation of residues and by-products through the production of new renewable products are investigate in order to improve the competitiveness of the entire production system. A variety of studies and investigations are carried out on biomass production, transformation processes and optimization of end-products use and recycling of by-products of oilseeds crops, lignocellulosic and autotrophic algae and yeast. The analyses on energy efficiency and environmental impacts are carried out on the whole agro-industrial life cycle. Furthermore, the best available technologies (raceway pond and photo-bioreactors) for the microalgae cultivation are compared in order to evaluate the eco-profile of a large scale biomass production: using wastewater as nitrogen source, carbon dioxide from industrial flue gases and renewable energies.



Valutazione dei benefici ambientali (es. analisi di LCA)

Environmental Impact Indicators (Embodied Energy Analysis (EEA), Energy Accounting (EA) and LCA has been applied to oleaginous crops: sunflower, rapeseed and tobacco. The results, according with our previous studies, show that the major

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impacts and uses of resources of the three crops are due to the production of mineral nitrogen fertilizers and diesel fuel. The comparison of the environmental impact of the three crops (LCA conducted with SimaPro 7.3.3) show that sunflower has the highest impact on most of the impact categories. Final results show that despite their high potential as sustainable energy feedstock, micro-algae are not yet competitive with the traditional oil crops in both economic feasibility and environmental impact.

A further important result is that the use of renewable technologies as photovoltaics and biogas self production could increase the competitiveness of micro-algae oil reducing its demand of non-renewable energy sources. This can reduce the costs of production of oil from micro-algae, allowing a cheaper and more efficient production of biofuel or value added crops in remote locations far from sources of electrical power.



Comparison among sunflower oil, rapeseed oil and micro-algae oil production processes (ReCiPe Midpoint (H) V1.04 / Europe ReCiPe H / Characterization).



Comparison with CED Method of three scenarios of algae oil production

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2A – Energy efficiencies and LCA studies on technologically advanced energy devices and grid system

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Aims

The project aims to achieve the primary goal of creating all the skills necessary for the manufacture of innovative three-phase distribution transformers (Medium Voltage /Low Voltage).

Results

This study wants to insert new types of MV/LV transformers with very high efficiency, not only in the European markets, but also in the American and Asian ones. The transformer which is currently being tested is based on a new concept type of ferromagnetic core, where the innovation lies in the construction of this element starting from a sheet of amorphous ferromagnetic material which, thanks to an automated construction system, manages to be wrapped inside the coils. The current architecture of the electrical system has been defined since its inception thanks to the invention of the transformer: this has allowed the development of electric generators in MT, the transfer in HT and end use both MT (industries) and LV.

The project wants to develop, on the one side an attractive product for the market (three-phase transformer with a continuous core in amorphous material), on the other an industrial process for the transformers realization. The production process will be based on the current machine providing a highly automated system, in which the intervention of an operator is limited to only some stages of preparation of the product. The model of the industrial machine (IMM), is composed of four stations, three reserved for the formation of cores and one for the removal of the completed transformer.



The three processing stations are functionally identical and consist of the same basic module developed by Newton (PIMM). The production process involves the construction of the three phase transformer in four distinct stages, each characterized by the formation of a specific part of the transformer.



Once completed the winding of the three ferromagnetic cores, the transformer can be subjected to a hardening phase if the resin applied on the surfaces if the tapes being the thermosetting resin, the transformer can be placed in an oven to effect polymerization if the resin itself and consolidate thereby between them the coils of the amorphous material.

The production process is completely different from the one currently used for the production of core laminations, and the solution developed will allow the lead partner to introduce a high degree of automation, so that the productivity of its plants can be significantly increased. Currently the production of this type of transformers is done with a low degree of automation, in fact the majority of the construction stages are done manually. The production system that the project intends to develop will guarantee certain costs for the production (having reduced the operators' manual intervention to a minimum), environmental benefits thanks to the use of the LCA (Life Cycle Assessment) and LCC (Life Cycle Costing) methodologies and a potentially improved productivity with time. The process will also help improve the standards of the product compared to the existing production processes, as it will be capable of a real series production.

Other important objectives of the project are the study and optimization of the resin from the chemical point of view, conferring it the specific characteristics required by the project as also in terms of solidification times. Other studies will consider the process of realization of the rolls, in particular the deposition of the resin. The final products of the project will be more samples of the pre-series of the transformer manufactured by the prototype of the production line.

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2A – Nanomaterials for enzymes immobilization

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Aims

The aim of this research is to address the catalytic properties of different enzymes supported onto nanomaterials for the bio-synthesis of new compounds for industrial applications.

Results

Immobilization of enzymes is advantageous for industrial application due to convenience in handling, ease of separation of enzymes from the reaction mixture and reuse, low product cost and a possible increase in thermal and pH stability. An important requirement for protein immobilization is that the matrix should provide a biocompatible and inert environment. Poor biocatalytic efficiency of immobilized



enzymes, however, often limits the development large-scale of bioprocessing to compete with traditional chemical processes. The result of immobilization, including the performance of immobilized enzymes, strongly depend on the properties of supports. Improvements of biocatalytic efficiency can be achieved hv manipulating the structure of carrier materials for enzyme immobilization. In recent decades, nanostructured materials have attracted much attention because of their unique properties and interesting applications. For example, electrospinning has emerged as a novel

tool to prepare fibers and membranes with high surface area-to-volume ratio in a cheap, fast and simple way.

For the same reason, novel ordered mesoporous materials like Santa Barbara Amorphous (i.e. SBA-15) has been synthetized in order to verify the application as enzyme carriers. Furthermore, the surface of these materials can be modified accordingly to the functional groups present on the enzyme surface to enhance the amount of supported enzyme and increase its activity.

Prepared and synthetized carriers have been analyzed by Scanning Electron Microscope, Transmission Electron Microscopy and Infra-Red Spectroscopy.

In particular, our attention has been focused on the study of the catalytic mechanism of laccase from *Trametes versicolor* (oxidative enzyme) and lipase from *Candida rugosa* (esterase/hydrolase enzyme) covalent immobilized onto the above mentioned carriers by the use of crosslinker molecules like glutaraldehyde.

Moreover, their potential use in organic synthesis has been investigated in order to compete with conventional synthetic methods. Indeed, immobilized enzymes have

been used in antibiotic production, drug metabolism, food industry and bioremediation.

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2A – Visible light activated carbon doped titanium dioxide for cleaning of olive mill wastewaters

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Aims

Study of the efficiency of the visible light activated Carbon doped Titanium Dioxide photocatalyst towards the olive mill wastewaters (OMW) compounds.

Results

Carbon doped titanium dioxide (CDT) was tested as catalyst for photodegradation of phenolic compounds of olive mill wastewater (OMW). The activation of the catalyst was triggered by exposure to visible light radiation. The cleaning effectiveness of this catalyst towards the polluted wastewater from olive oil industry was demonstrated by means of HPLC and UV-visible spectroscopy combined with phenol compound determination. The photodegradation activity was tested on systems having different initial concentration of phenols and in the presence of different amounts of CDT. By introducing a suitable parameter, namely the ratio between the amount of catalyst and the amount of total phenols Ti/TPh, it was demonstrated that the proposed degradation occurring in the presence of CDT particles under visible light radiation is marked enough to be directly appreciated with the naked eye. The decolorization is strongly associated with the removal of phenols. In fact, while bleaching the solutions, CDT successfully removed 70% of the phenols in 24 hours. HPLC analysis demonstrates that CDT was effective in degrading the higher part of the phenols of OMW.



Fig. 1: Above: the difference between TiO_2 and carbon doped TiO_2 in terms of light activation either UV or visible light. The difference of band gap energy from 3.2 to 2.3 eV is also highlighted. Below: OMW from the production of olive oil, the content of phenols and the photo-oxidation reaction obtainable in the presence of CDT is depicted.

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Fig. 2: Whitening of OMW in the presence of visible light activated CDT. HPLC chromatograms refer to the initial OMW phenolic fraction (upper chromatogram) and to the phenolic fraction after 23 hours of treatment. After 23 h almost all the representative phenolic species were removed from the water solution.

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2A – Physico-chemical analysis and characterization of ancient mortars and other archaeological materials

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Aims

The main aim of this project is to investigate, from the physico-chemical point of view, the materials coming from archaeological investigations.

Results

Within the framework of an archaeological and historical survey of the Medieval and Roman buildings of the Medio Volturno River area (in the Italian regions of Molise and Campania) conducted by the Laboratorio di Archeologia Tardoantica e Medievale (LATEM) of the University Suor Orsola Benincasa of Naples, we analyzed and characterized the samples of ancient mortars of about 25 historical sites of the area, dating from the 1st century B.C. to the 14th century A.D., taken from several different kind of buildings, with civil, religious, and military uses. The physico-chemical characterization of the mortars was carried out by X-ray powder diffraction (XRPD) with Rietveld refinement, for the quantitative determination of their mineralogical compositions, with subsequent validation by scanning electron microscopy (SEM) with energy dispersion spectroscopy (EDS). Moreover, thermo-gravimetric measurements (TGA) were performed to determine the water content of the mortars, and microscopic thin sections analyses were made to obtain information about their morphological and basic physical properties. The results of the analyses were mapped by our GIS system (Fig. 2), and compared with geological data of the area of interest to find the relation between the composition of the mortars and the typical minerals present in each area.





Fig. 2

We also found that, during the classical Roman period, the Vitruvius' suggestion of using "pure carbonate rock" was the standard practice, not only for the binder, but also for the aggregate part of mortars, in particular for public buildings, such as bridges and city walls. On the contrary, during the Middle Ages it was common to use other raw materials with lower percentage of carbonate rocks, such as feldspars and other volcanic minerals, typical of the region Campania areas, rich in volcanic sediments, and also some amorphous materials, such as ground bricks, and glassy volcanic stones. It is also frequent to find poor quality medieval mortars, because of the low quality of the raw materials from one side, and because of the often hurried binder preparation process, resulting in more friable mortars and, consequently, in less durable walls.

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2A – Organogels for the cleaning of artifacts

M.D. Pianorsi, M. Raudino, P. Ferrari, N. Bonelli, D. Chelazzi, R. Giorgi, E. Fratini, P. Baglioni

Aims

Synthesis and characterization of chemical organogels with tunable properties for the cleaning of artworks.

Results

Gels are particularly useful for the cleaning of works of art, as they allow the controlled delivery of cleaning fluids on solvent-sensitive substrates such as easel paintings. Owing to the presence of covalent cross-links between the polymer chains, chemical gels exhibit mechanical properties that allow their easy handling and their residue-free removal from artistic surfaces after the cleaning intervention.

MMA-based organogels obtained by solubilizing MMA in pure organic solvents (e.g. ethyl acetate, butyl acetate and metyl-ethyl ketone) and using a dimethacrylate crosslinker were prepared for the removal of historical varnishes from canvas painting samples. The macro- and mesoporosity of the gels have been characterized through Scanning Electron Microscopy (SEM) and Small Angle X-ray Scattering (SAXS). Moreover, a new organogel, based on MMA and MEK was specifically designed for the selective removal of aged wax layers from the surface of ancient (solventsensitive) inked paper. The new gel formulation was designed in order to improve on previous PMMA-based gels, which lacked the desired retentiveness, for extending their application also to paper substrates. To achieve this improvement, we systematically tuned the amount of cross-linker and monomer-solvent phase ratio used during the free radical polymerization of MMA in the MEK liquid phase, which allowed obtaining organogels with optimal characteristics in terms of retentiveness and mechanical properties (i.e. feasible handling and removal from the treated surface). The increased amount of cross-linker and the different solvent-monomer ratio used in the radical process, resulted in a decreased solvent content and mesoporosity of the gel network. In turn, this led to a slower and more gradual solvent release, both on porous and non-porous surfaces, as compared to the previous formulation (see left panel in figure). The PMMA-MEK organogels were applied on a 19th century inked document (see figure) to remove spots of paraffin wax that hindered the readability and aesthetic appearance of the artifact. The performance of the new systems (PMMA-MEK.3) was compared to that of the previous formulation (PMMA-MEK.1, PMMA-MEK.2). The gel formulation previously developed (which worked well on varnished canvas paintings) led to uncontrolled spreading of MEK and to the formation of tidelines on the paper surface (A1-2 in figure). On the other hand, the new PMMA-MEK.3 system allowed a safer and more gradual release of solvent on the paper surface, which led to the gradual swelling and detachment of the wax contaminant (B1-3 in figure).

After the cleaning intervention, the gel can be removed without leaving polymer residues on the surface as verified by ATR-FTIR.

Overall, this work validated the tunable synthesis of PMMA-based organogels as a process to produce versatile cleaning tools that can be used on different artistic surfaces, decreasing the risks of altering the original properties of the artifacts.

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2A – Chemical hydrogels for the cleaning of artifacts

N. Bonelli, E. Fratini, R. Giorgi, P. Baglioni

Aims

Removal of undesired materials from water-sensitive artifacts while avoiding solvents penetration. Formulation of semi-IPN chemical hydrogels.

Results

Nowadays, cleaning procedures on artifacts are mainly based on the use of pure organic solvents. This approach presents some drawbacks for both the object and the operator: solvents can easily penetrate within the porous matrix of the artifact and swell or solubilize paint binders and pigments; a second issue is due to the fact that most of the commonly used solvents are toxic. To avoid these problems, recently conservators are using some confining tools. Most of them are physical gels, such as *solvent gels* or polysaccharide based hydrogels. The first class leave some substantial residues on the surface after the treatment while the second class is fragile and does not offer a suitable control in the release of the cleaning agent.



Removal of grime from a tempera magra painting using a water-loaded semi-IPN p(HEMA)/PVP hydrogel.

This project is focused on two main points: limit the use and volatility of free solvents and avoid any gel residues by substituting physical gels with chemical gels. Chemical gels have strong gel cohesion due to covalent bonding between polymer chains and permit to load high amounts of liquid without undergoing gel solubilization. Chemical gels are versatile and can be functionalized to meet specific issues in conservation.

Cleaning water-sensitive artifacts (e.g. paper manuscripts, canvas paintings, etc.) is at present a problematic intervention in conservation, because the use of water and water-based systems (e.g. microemulsions) could interact strongly with the hydrophilic components of the artifact. Fiber swelling due to an excessive wetting of the fibers can cause mechanical stress or paint detachment. Chemical gels based on semi-interpenetrating polymer networks (semi-IPN) allow to obtain hydrogels that have suitable retention features for the cleaning of water-sensitive artifacts. Semi-IPNs are based on a polymer network that is formed in presence of an interpenetrating linear polymer. We have devised some formulations based on a poly(hydroxyethyl methacrylate) polymer network embedding linear chains of poly(vinylpyrrolidone). The resulting p(HEMA)/PVP hydrogels are high hydrophilic, their equilibrium water content (EWC) for different hydrogel compositions ranges from 72% to 87%.

Hydrogels are able to load water, o/w microemulsions and some pure solvents. By varying hydrogels composition the release/retention features can be tuned, making them suitable for different cleaning purposes.

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2A – Film forming PVA-based cleaning systems for the removal of corrosion products from historical bronzes

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Aims

Development of plasticized PVA-based polymeric systems loading complexing agents for the safe removal of alteration products from historical Cu-based alloys.

Results

Innovative poly(vinyl)alcohol-based film forming system, specifically devised for the controlled and selective cleaning of copper-based artifacts were developed.

Traditional cleaning procedures of metallic artifacts are commonly performed by mechanical and/or chemical methods. Both these methods present some limits related to both, the poor selectivity and invasiveness of the mechanical procedure, and to the scarce control over the reactions involved in the chemical approach.

In the case of copper-based alloys, the cleaning procedure is particularly delicate, it should aim at the complete removal of the defacing and harmful corrosion products of Cu(II) (copper carbonates, sulphates, chlorides, etc.) but preserving the underlying protective cuprite Cu(I) layer.

The proposed cleaning procedure consists in the application of a PVA-based polymeric solution able to form an elastic film, which can be gently peeled off from the surface upon drying. Plasticizers (different polyols) were added to the solution in order to obtain a final film with suitable mechanical properties to facilitate the peeling action, while the composition of the volatile fraction (water and ethanol) was adjusted in order tune both, the viscosity of the system and the time required for the film to form. Finally, a complexing agent (EDTA, chosen because of its good chelator performances and selectiveness for Cu(II)) was loaded in the polymeric dispersion.

The main advantage of this cleaning system consists in the simultaneous chemical and mechanical action, guaranteed by both, the presence of the complexing agent and the final removal of the film by peeling off.

The physico-chemical characterization of the system was carried out in order to investigate the kinetics of film formation, the variation in mechanical behavior of the system during drying, and the properties of the final polymeric films. The kinetics of film formation were studied by means of gravimetric and thermogravimetric methods (both scanning and isothermal) and rheology (both dynamic and rotational experiments) was used to investigate changes in mechanical behavior during evaporation of the volatile fraction of the system. The final films were characterized by means differential scanning calorimetry (DSC) and ATR-FTIR to evaluate the crystallinity degree, which is correlated to rigidity of the polymeric film. Moreover, the viscoelastic behavior of the system before and after the addition of a complexing agent solution was studied by means of rheological measurements.

The PVA70 formulation, containing 70% of volatiles fraction (55% H_2O and 15% ethanol) showed the best application properties in terms of manipulation (initial viscosity), evaporation kinetics (see left panels in figure, showing the temperatures of evaporation and kinetics of formulations with different water/ethanol ratios) and elasticity of the final film (related to plasticizer content). PVA70 was loaded with 3% w/w EDTA and used for the cleaning of artificially aged Cu-alloy samples and on a real cases study, the "Fontana dei Mostri Marini" by P. Tacca in Florence (see figure, right panel).

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2A – Calcium and barium hydroxide nanoparticles for the consolidation of wall paintings

R. Giorgi, G. Poggi, D. Chelazzi, P. Baglioni,

Aims

Consolidation of wall paintings with compatible inorganic materials.

Results

The consolidation and protection of immovable works of art, such as wall paintings, plaster and stone artworks can be successfully achieved by using dispersions of alkaline-earth metal hydroxide nanoparticles. Before the introduction of nanotechnology in the conservation field, synthetic organic materials were widely applied by conservators for consolidation purposes. Unfortunately, their presence on artistic substrates was shown to be detrimental due to the different physico-chemical properties of polymers with respect to the materials constituting the original artworks. On the other hand, alkaline-earth hydroxides exhibit high compatibility with many artistic and architectonic substrates and thus represent a valid alternative to the organic coatings. The nanosized structure of the applied crystalline phases, together with the dispersing medium, is a crucial factor for the efficacy of the consolidation: in fact, particle size influences their reactivity and penetration through porous matrices. Furthermore, particles polydispersity greatly affects their performance on substrates. For example, matrices to be consolidated often exhibit wide pores size distributions; in these cases the usage of suitable bimodal dispersions is advisable for the best consolidation.

It appears thus evident that the processes involved in the preparation of nanoparticles and their dispersion in carrier media, all play fundamental roles in determining the final effectiveness and applicability of these conservation tools. Synthetic pathways and peptization methods are both important to shape and finalize the particles down to the desired properties, so to meet the requirements of specific consolidation issues.

The same period during which the usage of polymeric coatings was very popular, saw the development of the first compatible consolidation method for wall paintings by Enzo Ferroni, who introduced several elegant solutions to solve the conservation issues following the disastrous flood of Florence, in 1966. In particular, the so-called Ferroni–Dini method, designed for the conservation of sulfate polluted wall paintings, consists in applying ammonium carbonate and barium hydroxide aqueous solution loaded on poultices, in a two-step procedure.

An improvement of this method is represented by the usage of a dispersion of barium (alone or in mixture with calcium) hydroxide nanoparticles, or, in other words, of a colloidal system instead of a solution. Recently, new formulations of barium hydroxide nanoparticles, alone or in combination with calcium hydroxide, have been successfully used for consolidation of degraded wall paintings, even in presence of large amount of salts.

Research Projects

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These methodologies are currently used for the consolidation of wall paintings in Italy and other countries, including Mexico (for the conservation of mesoamerican paintings in Calakmul, Tlatelolco, Mayapan, Cacaxtla, Cholula and, more recently, Ixcaquixtla), Sweden, Israel, and Denmark.

CTS company (Italy) is now distributing in several countries this nanomaterial, whose tradename is "Nanorestore®", produced at the CSGI laboratory. Nanorestore is the first chemical product based on nanotechnology, made available specifically to the conservator community.

More recently, CSGI have placed on the market a new class of commercial products named "Nanorestore Plus®" that are an updated version of the classic formulation "Nanorestore®". Nanorestore Plus® formulations are composed of calcium hydroxide nanoparticles dispersed in short-chain alcohols such as ethanol and 2-propanol.

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2A – Nanomaterials for the cleaning and pH adjustment of leather

D. Pianorsi, D. Chelazzi, M. Baglioni, G. Poggi, R. Giorgi, P. Baglioni

Aims

The development of a combined treatment for the cleaning and pH adjustment of leather.

Results

Leather has been used by mankind since ancient times, yet the preservation of this collagen-based material represents a challenge for conservators worldwide. Leather objects are made from mammalian skin and hide, which are then transformed into a material that is resistant to mechanical abrasion, microbial attack and heat. This is achieved through the tanning process, where either vegetable tannins or salts of metals (e.g. chromium, aluminum) are commonly applied to improve the stability of collagen. In particular, tannins have been used since Neolithic time to retard decay, and vegetable tanned leather was indeed one of the most important materials in Western and Mediterranean Europe until the end of the 19th century, when chromium mineral tanning gradually came into use. Tannins form a complex with collagen, mainly through hydrogen bonds between free amino side groups of the collagen protein and hydroxyl groups from the polyphenolic tannin molecules, as well as through hydrophobic bonds.

Leather artifacts in historical collections and archives are often contaminated by soiling, salts, biocontamination or coatings that alter their appearance and readability. Moreover, degradation is promoted by the presence of acidic compounds, either coming from manufacturing processes (tannery) or from the absorption of air pollutants such as sulfur and nitrogen oxides. Acidity increases the rate of hydrolysis of bonds within the collagen structure, reducing the polymer's structural integrity and eventually turning collagen into a gelatin colloidal solution. The tanning agents break down in turn under oxidative and acid hydrolytic conditions, forming products that can promote the degradation of collagen.

Both cleaning and pH adjustment of leather pose a great challenge for conservators, owing to the sensitivity of these materials to the action of solvents, especially waterbased formulations and alkaline chemicals. In this study the cleaning of historical leather samples was optimized by confining an oil-in-water (o/w) nanostructured fluid in a highly retentive pHEMA/PVP chemical hydrogel, which allows the controlled release of the cleaning fluid on sensitive surfaces. The chemical gel exhibits optimal viscoelasticity, which facilitates its removal after the application without leaving residues on the object. Nanoparticles of calcium hydroxide and lactate, dispersed in 2propanol, were synthesized and used to adjust the pH up to the natural value of leather, preventing too high alkalinity which causes swelling of fibers and denaturation of the collagen.

The gel, nanostructured cleaning fluid and nanoparticles dispersions were tested on both modern and historical leather samples. The modern sample was a vegetable tanned (sumac) leather made from calfskin. Leaves from sumac shrub (Rhus coriaria) were among the most important vegetable source for tanning leather. The sample was
tested as received. The first historical sample was the cover of a Luther Bible (1749 AD). The second historical sample was the cover of a Missale Romanum (Roman Missal, 1725 AD). The historical samples exhibited surface deposits of dirt, salts, or waxy (or lipid) materials, which needed to be removed. In the picture, the visual aspect of samples before and after cleaning and pH adjustment is depicted.

The treated samples were characterized using Scanning Electron Microscopy (FE SEM), and infrared spectroscopy (ATR-FTIR). The analytical assessment validated the use of tools derived from colloid and materials science for the preservation of collagen-based artifacts.

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2A – Nanocomposite materials for the consolidation and strengthening of cellulose-based artifacts

G. Poggi, R. Giorgi, D. Chelazzi, P. Baglioni

Aims

Development of a nanocomposite material for the consolidation and concomitant pH adjustment of cellulosic works of art and artifacts.

Results

Two are the main issues need to be solved if the conservation of degraded fibrous material-based artifacts is concerned. Firstly, a mechanical reinforcement of artifacts is usually needed to ensure, for instance in the case of paintings, that the paint layer or decoration keeps its integrity. Moreover, pH buffering is needed to prevent acidic degradation that is inherent to natural materials. It has been recently shown that these two issues are related. As a matter of fact, the acidity of canvases made of natural materials is generally of concern as it can lead to loss of mechanical properties and deterioration of canvases based on natural materials in less than 100 years. The stability of synthetic canvases is even less known than that of canvases of natural origin. This problem dramatically concerns also jute, which becomes quite acidic in a faster way than linen, and paintings done on this type of canvas become more brittle. Therefore, the main areas for which both these issues are very relevant are conservation of modern and contemporary canvas paintings, as well as polymateric works of art using other types of fibrous supports such as paper. In fact, paper is also subjected to the same degradation mechanisms above described.

The application of glue and the attachment of a new canvas on the back of the painting, i.e. the lining, is traditionally used for the consolidation of canvases. However, although inevitable for the most degraded canvases, lining should to be avoided due to its invasiveness, because it hides the original canvas and is very resource-intensive.

Therefore, the goal within the EU Project NANORESTART is to develop materials for the mechanical strengthening of canvases of modern/contemporary paintings. The development and use of nanocellulose in combination with nanoparticles and cellulose derivatives could ensure the consolidation of fiber-based materials using almost entirely natural materials. The choice of these materials is due to the high compatibility of the proposed treatments with the original fibrous support, which is essential from the conservation point of view.

Mechanical tests on not aged and aged reference samples could be used to assess the consolidation efficacy of the proposed consolidation treatments before testing on real case studies.

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2A – Nanotechnology for the deacidification of cellulose-based works of art

G. Poggi, R. Giorgi, P. Baglioni

Aims

Deacidification of paper, manuscripts and wooden objects by means of alkaline earth metal hydroxide nanoparticles.

Results

Among the treatments used for the preservation and conservation of cellulose artistic substrates, deacidification represents the most diffused method, considering the primary role of acid-catalyzed hydrolysis in the degradation of cellulose-based works of art. In fact, almost every paper sheet produced in the past four centuries may be a carrier of potentially hazardous acid compounds that could initiate a degradation of the paper itself. For example, iron gall ink, obtained from the reaction between gallic acid and ferrous sulfate, leads to the formation of sulfuric acid. Moreover, "alumrosin" sizing, introduced in the first decades of 1800 requires the usage of the two reagents, both extremely acidic, directly added to the stock before paper was formed. In the case of canvas, recent measurements made in the EU-PROPAINT project have shown that levels of trapped organic acids within a frame enclosure of easel paintings exceed recommended threshold levels of $1000\mu g/m3$ and could cause long term damage. In addition to that, also archaeological wood can also be corroded by acid products, as in the case of the Swedish warship Vasa, whose preservation is probably one of the most challenging tasks that conservators are facing these days.

Carbonates and hydroxides of alkaline earth elements, such as calcium and magnesium, are usually selected for the deacidification of cellulose-based artworks due to their high compatibility. Recently, the contribution of colloids and materials science to the conservation framework has lead to the development of innovative solutions capable of overcoming the main issues of traditional methods. In particular, dispersions of alkaline nanoparticles, mainly calcium and magnesium hydroxide in non-aqueous solvents, have been proposed as efficient deacidifying treatments for cellulose-based works of art, such as paper, manuscripts and archaeological wood.

These nanoparticles, due to their high reactivity, provide a stable neutral environment by rapidly turning into mild alkaline species (carbonates). This will have the effect of hampering the β -alkoxy elimination, i.e., the alkali-catalyzed degradation of strongly

oxidized paper that may be associated with the application of traditional deacidification methodologies, especially when aqueous methods are used. Moreover, low polar solvents offer good wetting properties without damaging cellulose fibers whilst ensuring a homogenous distribution of particles within the artworks supports.

Recently, a new method for obtaining calcium hydroxide nanoparticles has been developed, based on a solvothermal reaction at high pressure and temperature. The main advantage of the synthetic procedure relies in the possible future up-scale of the process, with great benefits in term of costs. For the production of these nanoparticles, calcium metal and short chain alcohols are mixed in order to obtain a calcium alkoxide, which turns to hydroxide after the addition of water to the reaction bulk. For deacidification purposes, two dispersions are usually prepared, starting from ethanol and n-propanol. The effects of deacidification with calcium hydroxide nanoparticles have been investigated. In particular, artificially acidified paper and canvas samples and wood from the warship Vasa have been deacidified by using calcium hydroxide nanoparticles, which homogenously penetrates into the substrates, increasing the resistance of cellulose to ageing.

As a results of research efforts in the field of the conservation of paper and wood, CSGI have recently placed on the market a new class of commercial products named "Nanorestore Paper®", designed for the deacidification of cellulose-based materials. Nanorestore Paper® formulations are composed of calcium hydroxide nanoparticles dispersed in ethanol and 2-propanol.

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2A – A stabilizer-free nonpolar dispersion for the deacidification of contemporary art on paper

G. Poggi, R. Giorgi, P. Baglioni

Aims

The preparation and synthesis of non-polar dispersions of alkaline-earth metal hydroxide for the deacidification of modern inks documents.

Results

The preservation of cellulose-based works of art is threatened by the presence of acidity within the substrates, native, i.e., due to the papermaking process, or developed upon aging. The depolymerization of cellulose catalyzed by acidic compounds leads to a decrease in the mechanical properties of the artworks. Many strategies for hampering the acid-catalyzed degradation of cellulosic substrates have been developed in the past; unfortunately, few of them can be safely used on contemporary artworks, drawings or archival materials.

The use of paper started to change in the middle of 20th century, moving from a simple support for studies or sketches to being the heart of autonomous works, at time torn, burnt, folded, perforated, twisted or creased. This is the case of Simon Schubert, Kiki Smith or Stefano Arienti artworks. At the same time the world of art has seen the arrival of a large number of new media, such as acrylic and vinyl resins, pressure sensitive adhesives, ballpoint and felt-tip pens and markers. The same pens and markers used by contemporary artists can be found in manuscripts and archival documents. All of these media and techniques are rarely compatible with traditional restorative procedures. This makes the conservation and restoration of the wide field of contemporary drawings and archival documents unexplored. In particular, few are the available deacidification treatments that can be safely used on contemporary drawings or contemporary art on paper, as well as on contemporary documents and manuscripts.

A deacidifying dispersion of calcium hydroxide in cyclohexane has been prepared starting from alkaline nanoparticles obtained via a solvothermal reaction. The most interesting feature of this formulation is that a stabilizer is not required for the preparation of the dispersion, differently from other commercial nonpolar products. Cyclohexane is a colorless, nonpolar, and volatile liquid that allows fast and simple applications by spraying, respectful of the original artist's technique, as shown in the image reported below.

In order to evaluate the efficacy of this $Ca(OH)_2$ nanoparticles dispersion in cyclohexane, mockups were prepared on acidic paper using ballpoint pens.

The protective action arising from the applied treatment was evaluated upon artificial aging, measuring cellulose viscosimetric polymerization degree (DPv), cellulose pyrolysis temperature, samples pH, and colorimetric coordinates. The promising results obtained on mockups led to the application of this innovative formulation on a series of drawings from a private collection, opening the way for the treatment of such an important field of contemporary arts. Reflectance Transformation Imaging (RTI), a computational photographic method that captures the surface shape of artifacts in a noninvasive way, was used to evaluate the compatibility of the newly developed cyclohexane dispersion with burnt, perforated and creased paper.

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2A – Amphiphile-based nanofluids for the removal of organic coatings from works of art

M. Baglioni, D. Berti, E. Carretti, L. Dei, D. Chelazzi, R. Giorgi, P. Baglioni

Aims

Development of innovative, effective, safe and environmentally-friendly systems for the cleaning of painted surfaces.

Improvement of the available formulations with the inclusion of degradable (biodegradable, labile, cleavable) surfactants, which should solve the residues' issue.

Results

The removal of undesired material from the surface of a work of art has always been one of the most important and delicate operations in the conservation of cultural heritage. The availability of a great choice of pure organic solvents at first opened up new perspectives for cleaning operations. Nevertheless nowadays, most organic solvents are not the preferred option, in view of their poor-controlled action, their toxicity and the disposal and recycling concerns. Surfactant-based aqueous nanostructured fluids, such as micellar solutions and microemulsions, represent the most effective, safe and selective cleaning media currently available for cleaning operations in the conservation of cultural heritage. Due to their nature, these systems can be used to remove oily grime or hydrophobic substances from hydrophilic surfaces, as it is the case of polymer removal from wall paintings and stones. During last two decades the effectiveness of microemulsions and micelles in removing polymers from painted surfaces was thoroughly demonstrated.



Since the removal of wax spots from fresco paintings by Masaccio, Lippi and Masolino (Brancacci Chapel, Basilica del Carmine, Florence), which represented the first example of microemulsion application to conservation of cultural heritage, their use was extended to the removal of organic coatings (synthetic polymers, natural and synthetic varnishes, adhesives, modern paints) from wall paintings, easel paintings, stone, wood, paper and leather.

The main issue that still needs to be addressed with these systems is that surfactants may remain on the treated surfaces as a residue (which, nonetheless, can easily

washed away by rinsing with water). In fact, surfactants are the only non-volatile chemicals included in these formulations. Thus, using surfactants that spontaneously degrade to harmless volatile compounds would be a major advancement of this methodology. We recently moved our focus from ionic surfactants to nonionic alcohol ethoxylates, which possess interesting (bio)degradability properties, and we are currently studying new classes of surfactants, such as cleavable pH sensitive autodegradable surfactants.

Interesting results are being obtained using these innovative surfactants in new nanofluids.

As a result of these research efforts, nanofluids for the cleaning of cultural heritage have been made available to conservators and restorers as commercial products under the trademark of Nanorestore Cleaning[®].

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2A – Nanostructured fluids for the conservation of cultural heritage: understanding the mechanism of organic coatings removal

M. Baglioni, D. Berti, C. Montis, M. Raudino, M. Bonini, P. Baglioni

Aims

Understanding the mechanism of interaction between polymer coatings and nanofluids will contribute to improve cleaning formulations in the field of conservation of cultural heritage, and, besides having some scientific relevance from fundamentals standpoint, it may open new perspectives on different applicative fields.

Results

The removal of undesired material from the surface of a work of art is one of the most important and delicate operations in conservation of cultural heritage. In this context, nowadays, neat organic solvents often are not the preferred option, in view of their poor-controlled action, their toxicity and the disposal and recycling concerns. Surfactant-based aqueous nanostructured fluids, such as micellar solutions and microemulsions, represent the most effective, safe and selective cleaning media currently available for cleaning operations in the conservation of cultural heritage. Due to their nature, these systems can be used to remove oily grime or hydrophobic substances from hydrophilic surfaces, as it is the case of polymer removal from wall paintings and stones. During last decade the effectiveness of microemulsions and micelles in removing polymers from painted surfaces was thoroughly demonstrated.



Most recently, a major effort has been spent in order to investigate the mechanism of polymer removal from porous substrates using nanofluids. The rules of classical detergency seem to not fully address the polymer removal mechanism, and a complete and satisfactory description of the process is still missing. Scattering techniques and imaging investigations, such as confocal laser scanning microscopy, are being combined in order to obtain a clearer picture of the cleaning mechanism.

In particular simple ternary mixtures of water/solvent/surfactant at different concentrations were examined, in order to clarify the role of each component in the

formulations, in the interaction with thin films of Paraloid B72 (a ethyl metacrylate/methyl acrylate 70:30 copolymer). Propylene carbonate and methyl ethyl ketone were selected as solvents, while nonionic CiEj surfactants and SDS were considered as surface-active agents.

The results are indeed a step forward in understanding the interaction mechanism between nanofluids and polymeric films at the micro- and nano-scale. A dewetting process is promoted by aqueous nanofluid, which seems to be strongly influenced by the presence, concentration and nature of the surfactant in the cleaning system. The role of micelles or supramolecular aggregates in this context is currently under investigation, as well as the dependence on the thickness of the examined polymer films.



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2A – Nanofluids and chemical hydrogels for the selective removal of overpaintings and undesired graffiti from street art

M. Baglioni, R. Giorgi, P. Baglioni

Aims

Removal of graffiti and overpaintings from street art, or, more in general, contemporary art, cannot be performed using available traditional methodologies; therefore selective removal can be achieved combining highly retentive hydrogels and nanofluids.

Results

The removal of graffiti from paintings that must be preserved is a particularly challenging and relatively new issue in conservation of cultural heritage. This is the case of contemporary street art (by unconventional contemporary artists, such as Banksy or Blu) jeopardized by tags, signs and writings. In these conditions, the cleaning action must be extremely selective, as the binder of the undesired paint is likely to have a very similar chemical nature to the one of the underlying original painting.



To this aim, in the frame of an Horizon 2020 EU-funded project named Nanorestart, nanostructured fluids, such as micelles and microemulsions, either neat or combined with highly retentive chemical hydrogels was proposed and it is here reported as a selective and controllable cleaning system for the removal of graffiti and overpaintings from street art. The semi-interpenetrating polymer networks-based hydrogels (SIPN) here proposed are composed by a tridimensional network of

poly(hydroxyehtyl methacrylate)/N,N'-Methylene bisacrylamide (pHEMA/MBA), interpenetrated by a high molecular weight poly(vinyl pyrrolidone) (PVP). These hydrogels have been shown to be particularly suited to limit the cleaning action to the surface layers of the treated area. pHEMA/PVP hydrogels can be loaded with water, some polar solvents, or with aqueous nanostructured fluids (hereafter, shortly, "nanofluids"), composed by eco-friendly, volatile or auto-degradable compounds, which ensure a residue-free and environmentally compatible cleaning intervention. The studied formulations were structurally characterized by means of scattering techniques and their phase diagram was investigated. Then, they were tested on laboratory samples simulating street art paintings covered by graffiti. The samples were prepared by overlapping different paints in various combinations. The paints included in this study include acrylic, vyinl and alkyd binders, while several colors were tested. The outcome of cleaning tests was investigated by means of visual, photographic and microscopic observation, while micro-reflectance FT-IR spectroscopy was performed on the treated area before and after the application of the cleaning systems, in order to gather information about the chemical composition of the surface, searching for possible residues of the removed paint layer. Setting up application times and performing careful and delicate mechanical action were found to be key factors when removing overpaintings having the same binder as the original paint layer. However the removal of acrylic (or vynil) paints from other acrylic (or vynil) paints was achieved with minimum stress for the original paint layer. Microscopic observation and FT-IR analysis of the treated areas confirmed the good results of the cleaning tests.

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2B – Effect of mechanical energy on solid state synthesis of Ternary Oxides

V. Berbenni, G. Bruni, C. Milanese, A. Girella, A. Marini

Aims

Through different analytical techniques, the formation reactions of some technologically interesting ternary oxides are followed.

Results

The mechanism of $Bi_4Ti_3O_{12}$ formation starting from the two constituent oxides has been studied. Starting from a physical mixture, a solid-state reaction occurs between the two oxides that leads at ≈ 700 °C to a mixture of the two ternary oxides $Bi_{12}TiO_{20} + Bi_4Ti_3O_{12}$ along with unreacted precursor oxides. At $T \approx 830$ °C $Bi_{12}TiO_{20}$ reacts with TiO₂ forming $Bi_4Ti_3O_{12}$ and, finally, at $T \approx 850$ °C, the residual $Bi_{12}TiO_{20}$ undergoes the peritectic reaction that produces $Bi_4Ti_3O_{12}$ plus a liquid phase. However, the formation of $Bi_4Ti_3O_{12}$ is not complete at temperatures as high as 900 °C. Starting from a mechanically activated mixture, the intermediate $Bi_{12}TiO_{20}$ only forms as a minority phase at a lower temperature (T ≈ 550 °C), and then it rapidly reacts to give $Bi_4Ti_3O_{12}$. No trace of the peritectic reaction is found in the case of the activated mixture. The complete formation of $Bi_4Ti_3O_{12}$ can be obtained by 3-h annealing of the activated mixture at $T \ge 650$ °C. The heat capacity of the product phase $Bi_4Ti_3O_{12}$ has also been measured in the temperature range 50-300 °C.

Many synthesis procedures have been worked out to prepare CaSnO₃. A great deal of them resort to the classical ceramic method that implies a very high temperature treatment (1300-1500°C) of the component oxides mixture. To avoid such high temperature treatment, many alternative routes have been proposed. In this paper stoichiometric mixtures of Ca citrate tetrahydrate and Sn(II) oxalate have been mechanically activated by high energy milling. The reactions taking place in the mixtures during annealing have been studied by coupled TG-DSC measurements, XRPD and diffuse reflectance FT-IR spectroscopy. It has been established that the stage of mechanical activation allows the synthesis to be completed by 3 h-annealing at 850°C.

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2B – New cathode materials for technological applications

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Aims

Characterization and optimization of the physico-chemical properties of materials for electrochemical applications, to put into evidence the relationships among properties, synthesis method and doping.

Results

We investigated in detail a series of undoped and doped compounds that find application as cathode for lithium batteries. The investigation involves the structural and microstructural studies, and the physico-chemical characterization of pure and doped ceramic compounds and oxides solid solutions. Conventional and synchrotron X-Ray diffraction data are used to study the structure stability with cell cycling, the cations and doping ions distribution in the cell framework, and to quantify the possible impurity phases formed in the synthesis process. The results, obtained by the combined use of several structural and spectroscopic techniques, are useful to explain the materials properties. The investigated cathodes compounds belong to the Li-Fe/Mn/Co-Si-O and Li-Mn/Ni-O systems. For the preparation of pure and substituted compounds, different synthesis routes were used, to optimize the material properties for its technological application.

Wide interest has been devoted to the study of lithium transition metal ortho-silicates Li_2MSiO_4 (M = Co, Mn, Fe). As cathode materials in Li-ion batteries they offer the possible extraction of two Li ions per formula-unit and a particularly stable anionic framework, thanks to the strong Si-O chemical bonds, thus promoting both higher charge-discharge capacities and longer cycling life. Nevertheless, the presence of different polymorphic forms, the defects formation, and the easy segregation of impurity phases during the synthesis influence the Li diffusion and its intercalationde-intercalation mechanism, thus affecting the electrochemical performances. In this frame, we investigated the influence of the synthesis procedure on the structure, defects formation and purity of Li₂FeSiO₄, Li₂MnSiO₄, Li₂Fe_{0.5}Mn_{0.5}SiO₄ and Li₂(FeMnCo)SiO₄ by the combined use of structural, spectroscopic and magnetic techniques. More interestingly, we studied the structural changes of the cathode material during cycling by in-situ and ex-situ X-ray conventional and synchrotron diffraction data. Moreover, we reported, for the first time, the successful preparation of thin films of lithium iron and manganese orthosilicates cathodes, deposited by RF sputtering, to be used in lithium microbatteries. The experimental evidence of the voltage variations during the charge-discharge of Li₂FeSiO₄ has been explained by density functional theory calculations.

Among the high-voltage cathode materials for Li-ion batteries, the Si doped $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ spinel compound has been prepared and characterized. We demonstrated that the successful substitution of the silicon ions on the tetrahedral site of the cationic framework is obtained for silicon content lower than x=0.15 in $\text{LiNi}_{0.5}\text{Mn}_{1.5-x}\text{Si}_x\text{O}_4$. The silicon substitution plays a favourable role in the structure stability and lithium diffusion, thus improving both charge-discharge capacities and cycling performances of the cell.

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2B – Synthesis and characterization of nano-biomaterials

M. Bini, D. Capsoni

Aims

Synthesis and characterization of pure and doped Hydroxyapatites and Zinc ferrites to optimize their biomedical applications.

Results

Due to its compositional similarity to mineral bone, hydroxyapatite (HAp), Ca₁₀(PO₄)₆(OH)₂, has been widely investigated for its possible use to promote bone ingrowths when used in orthopedics applications. More studies showed that the traditional HAp materials lacked the ability to induce osteogenesis; this problem can be overcome by proper doping/substitution with different cations on Ca and P sites. In particular, silicon has been demonstrated to be essential to the normal growth and development of bone and cartilage, and can enhance osteoblast proliferation and differentiation, as well as improve collagen production. Also the manganese substitution plays a favorable role in the hydroxyapatite applications. A few is known on the possible role played by Mn/Si co-substitution on the hydroxyapatite performances. Nanocrystalline pure and Mn/Si co-substituted hydroxyapatite were synthesized by different procedures and the samples have been characterized by structural and spectroscopic techniques. The Mn substitution occurs on the Ca(I) crystallographic site of the Hexagonal crystal lattice, while Si ions occupy the P site. SEM analysis confirms that all the samples are of nanometric particle size and the distribution maps of the elements demonstrate that Ca, P, Si and Mn are homogeneously distributed in the samples. The as-synthesized samples were soaked in SBF (simulated body fluid) solution to evaluate their bioactivity. ICP analysis showed a good in-vitro bioactivity and a satisfactory biocompatibility.

A study of magnetic Zinc ferrites nanoparticles has been also undertaken, due to the numerous applications that they can find in various fields such as electronic devices, electrodes for batteries or sensors, as well as in the biomedical field where they can be used as contrast agents (CAs) in magnetic resonance imaging (MRI). Our research focuses on their magnetic hyperthermia application (MHF). The magnetic property of interest for this application is called superparamagnetism, that is present when the nano particles are so small that can be considered as a single magnetic domain. In this frame, we investigated zinc ferrite nano-powders with a nominal composition of ZnFe₂O₄. They are magnetic materials with cubic spinel structure and their properties are strongly influenced by the materials' composition and microstructure, which are sensitive to the preparation methodology and also to the doping. Thanks to their superparamagnetism property, particularly prominent when in nanometric dimension, $ZnFe_2O_4$ ferrite nanoparticles are arousing a great interest for magnetic hyperthermia application. In order to improve the magnetic properties of ferrites different methods of synthesis and various types of doping have been tried. The synthesized samples were thoroughly characterized by XRD with Rietveld structural refinement, SEM/EDS, Micro-Raman and FT-IR spectroscopy. The magnetic properties were determined by SQUID magnetometry by collecting hysteresis loops and the magnetization dependence on temperature was determined in zero field cooling and

field cooling regimes. With these characterization techniques, it was shown that the samples obtained are actually nanometric and do not present significant impurities amount. The dopants are easily inserted in the spinel structure and are homogeneously distributed in the nano-particles. The magnetic measurements allowed us to demonstrate that the samples show a pronounced superparamagnetism, that makes them suitable to be employed in MHF.

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2C – Chemical Characterization and Antioxidant Properties of Olive Pomaces and Olive Leaves

C. Rossi, G. Tamasi, C. Bonechi, S. Lamponi, A. Donati, A. Magnani

Aims

The study of antioxidant chemical and biological properties are increasing on interest in the last years. The presence of oxidizing species and/or free radicals in foods, reduces its nutritional value and sensory quality due to oxidative reactions in addition to doing damage to human health, for example provoking mutations in DNA. Antioxidants can prevent these reactions via hydrogen atom transfer, electron transfer mechanism or transition metals chelation.

Results

This present study reports the characterization and determination of selected antioxidant properties in olive fruit, extravirgin olive oil (the primary product) and pomace (by-product) samples from the harvesting/production 2013 (one sample, preliminary test), 2014 and 2015. Olive leaves from the pruning process 2013 have been also investigated.

All the samples have been previously lyophilized and extracted via hydroalcoholic mixture (EtOH/H₂O, 80/20, v/v). The extracts have been characterized as regards the antioxidant activity through the TEAC (Trolox Equivalent Antioxidant Capacity) and DPPH assays, as well as the analysis of the total polyphenol content (Folin-Ciocalteu method). Selected polyphenols, quercetin, rutin, naringenin, luteolin, epicatechin, kaempferol, and chlorogenic acid, p-coumaric, caffeic and ferulic acid, have been determined quantitatively via HPLC/MS technique. Analysis was ended by analyzing selected metal ions: Na, K, Mg, Ca, Cu, Mn, Zn in the hydroalcoholic extracts as well as in mineralized samples

The hydroalcoholic extracts have been also characterized as regards the viability assay on 3T3 fibroblast cells, showing no toxicity up to 2.5% of extract in the culture medium, while a 5% becomes toxic. This effect can result from the known pro-oxidant activity of polyphenols.



Fig. 1: Kinetic of TEAC values for pomace harvesting 2013 (180 h, P13 lyophilized and extract, EtOH absolute). The extract was kept at different conditions:- 20 ± 1 , 4 ± 1 e 20 ± 2 °C. Confidence interval, 95%

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2C – Chemical characterization of peaches and nectarines

C. Rossi, G. Tamasi, C. Bonechi, G. Leone, A. Donati, A. Magnani

Aims

Chemical characterization of vegetables for food use, and their extracts rich in antioxidant and bioactive components, has increasing attention and efforts on investigating. Particular attention has being devoted to use different and complementary analytical techniques, in order to determine and quantify the key phytochemical compounds. The data can then be interpreted by applying a chemiometric approach.

Results

This study has been conducted on samples of yellow fleshed peaches (Prunus persica L. Batsch; cultivars: RomeStar, ZeeLady) and yellow fleshed nectarines (Prunus persica L. Batsch, var. Nectarina; cultivars: Venus, Nectaross) from two geographic areas of Southern Italy, "Piana di Sibari" and "Piana di Metaponto", located on the Ionian coast of Calabria and Basilicata regions.

The thermogravimetric analysis (TGA) has shown a similar chemical composition of samples having 88±1% water content, 5.4±0.8% sugar content, 1.8±0.2% fibrous content and the remaining 4.8±0.6% associated to minerals. Finally, the rheological analysis revealed a similar consistency of samples (reasonable with a similar maturation stage), and characterized by a greater elastic than viscous component. The measurements of the antioxidant activity (TEAC method) and total polyphenols (Folin-Ciocalteu method) for hydroalcholic pulp extracts, have shown values with comparable trend for the two varieties of nectarine, while in the case of peaches, showed more changeable values. The HPLC-MS analysis of pulp extracts, allowed the identification and quantification of selected polyphenols: chlorogenic and neochlorogenic acid and quercetin glycosides (isoquercetin and rutin), showing a predominant relative distribution of the two hydroxycinnamic acids (Figure 1a), in agreement with the antioxidant activity (and total polyphenols). ¹H-NMR spectra revealed the presence of sugars (sucrose, α - and β -glucose, α -xylose, β -Dfructopyranose) among the main constituents of pulp extracts, presenting only minor differences in chemical shift and peaks intensity between samples, in agreement with a very similar chemical composition between peaches and nectarines. The Principal Component Analysis (PCA), obtained by statistical processing of the ¹H-NMR data, showed the presence of two outlier samples (ZeeLady-Peach and Nectaross-Nectarine) in agreement with different chemical compositions (particularly high values of hydroxycinnamic acids). Furthermore, Cluster Analysis (CA) showed the grouping of samples on the basis of cultivars (nectarines and peaches) with a 60% significance level. The FTIR-ATR measurements on lyophilized samples of pulps and skins has been also performed, confirming the presence of characteristic bands of -COOH groups of organic acids, -OH groups of sugars, phenols, water, and peptide groups (NH-CO) (Amide bands I, II and III) of proteins. On comparing the skin and pulp FTIR-ATR spectra, more intense absorption bands in the region 1800-1500 cm⁻¹ have been found on exocarp samples, attributable to cyanidins, while more intense

absorption bands corresponding to sugars between 1200-800 cm⁻¹ have been observed in mesocarp samples. Finally, ToF-SIMS analysis has been carried out, confirming the presence of cyanidin and phosphatidylcholine in the skin of peaches and nectarines, and cyanidin, phosphatidylcholine, oleic acid and coniferyl alcohol in the skin of seeds. The CA obtained from the skins of the seeds, constitutes a viable option for the geographic characterization of peaches and nectarines (Figure 1b).



Fig. 1: (a) Relative distribution of hydroxycinnamic acids on hydroalcoolic pulp extracts (HPLC-MS analysis); (b) Cluster analysis from ToF-SIMS data from skin of seed samples.

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2C – A multidisciplinary project for the study of historical landscapes: new archaeological and physicochemical data from the "Colline Metallifere" district

A. Donati, V. Volpi, L. Dallai

Aims

The aim of this work is to present some results obtained by a combinedmultidisciplinary approach to the study of a territory located in the southern part of Tuscany, the "Colline Metallifere" district. In this paper we are focusing particularly on the use of chemical analyses (pXRF) on crucial historical areas. The considerable amount of information retrieved and the unquestionable value of the data obtained by the pXRF analyses are now opening new fields to the use of the portable instrument.

Results

In the last years the Colline Metallifere district (southern Tuscany) has become a multidisciplinary study area in which a combined archaeological, geological, and environmental approach is providing new interesting evidences for the reconstruction of historical landscapes. Extensive surveys on territorial samples have been carried out to define the main aspects of mining exploitation and metal production; the data collected have been processed with the aim of defining a broad picture of the territory both from an archaeological, geological and environmental perspective.



In order to get the maximum amount of useful information, a combination of underground surveys, fieldworks and XRF analyses on fluvial sediments and soils explored the technical aspects of the production and the environmental impact of ancient mines. From the different case studies combined archaeological and physico-chemical data (pXRF in particular) are gruadually building up a solid database that is helping in defining the historical outlines of the Colline

Metallifere landscape.

In the case study of Montieri village the environmental data collection helped to define, on a smaller scale, the topographic limits of a large slag area, very well known from historical descriptions, nowadays partly covered by the standing town of Montieri. The slags are the result of the ore extraction and metallurgical processes that went on around Montieri's village during the Medieval period. The place, as said above, has been in fact in that historical phase an important mining and metallurgical center, and numerous silver mines are still partly visible in the surrounding hills and have been identified by the archaeological surveys.

To estimate the extent of this pile of slag with an initial level of topographical approximation, a large-scale screening was conducted on the river sediments, using the natural leaching process of contaminated soil as a guide. In the case in hand, lead was used as the "tracer" element; indeed, lead is very closely connected with silver



extraction (production from silver-bearing galena). Along the streams it was made a systematic stream sediment sampling for the laboratory analysis through the Atomic Absorption Spectroscopy (AAS) technique.

Results from the analyses showed a high concentrations of Pb on the central rivers compared with the peripheral ones. This indicates that the contamination originated from an area approximately definable (1A). The subsequent level of refinement has included chemical measurements of the soil; this has led us to define with greater precision the area where the slag probably accumulated. The area that can be calculated on the basis of these figures is around 7,500 mt² with a depth of around 4 mt in the southern extremity to a few dozen cm in the northern extremity (1B).

This research is important to determine some important chemical feature for a better understanding of the local historical mining context. In particular it is crucial to find out on the one hand some productive characteristics that can help in defining the amount of mineral worked and, consequently, of metal produced. On the other hand, behind the archaeological aspect, it is useful to verify the spread of contamination and to understand to what extent the presence of metallurgical slags has affected the local environment, providing general indications on the toxic elements speciation in the area.



Fig. 1: A) Montieri's vector topographic map. It shows the results of Atomic Absorption Spectroscopy (AAS) analysis of Pb distribution in the river sediments. The darkness of blue color is proportional to the concentrations of Pb. B) The concentration of lead in soil slag heap. The polygon represent the waste area.

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2C – Identification of catalytic protein radicals in LRET mechanism of peroxidases and variants

M.C. Baratto, A. Sinicropi, R. Basosi, R. Pogni

Aims

A combined spectroscopic and computational approach, together with site-directed mutagenesis studies, enabled to identify and characterise catalytic different protein radicals formed through LRET pathways in novel peroxidases.

Results

Peroxidases, a lignin-degrading system, are able to oxidize high redox potential aromatics via exposed protein radicals. Direct detection of a protein radical (Trp radical) in a ligninolytic peroxidase as a catalytic site, was obtained, for the first time by our group, in Pleurotos eryngii and Bjerkandera adusta Versatile peroxidases (VP). The role of protein radical intermediates in the catalytic cycle was studies by multifrequency EPR and identified in the Trp164 site in the P. eryngii VP. In a new Lignin Peroxidase (LiP), recently found in the Trametopsis cervina, it was found that the conserved catalytic tryptophan lacks and it contains one tyrosine residue (Tyr181) at a position where tyrosine residues were never found in other LiP and VP sequences. Low temperature EPR of the peroxide-activated T. cervina LiP successfully detected a protein radical at Tyr-181. These results provide the first structure-function information on the only ligninolytic peroxidase described to date that has a catalytic tyrosine. A new peroxidase, DyP dye-decolorizing peroxidase has been recently tested and characterised. DyPs are widely distributed in fungi, bacteria and archea. The terms "dye-decolorizing" derives from the ability to decolorize and degrade xenobiotic anthraquinone and azo dyes. The catalytic mechanism of DyPs is similar to that of classical peroxidases, where the resting enzyme undergoes a two-electron oxidation by hydrogen peroxide to Compound I (CpI). The activated enzyme is then reduced back by two substrate molecules to the resting state via the Compound II. Different

from other fungal peroxidases in the distal side arginine and aspartic residues contribute to the heterolytic cleavage of H_2O_2 to form CpI. AauDyP possesses seven Tyr and four Trp residues as potential sites to active different long range electron transfer pathways (LRET).

To oxidise bulky substrates, a LRET pathway was also suggested for AauDyP. Simulations using PELE (Protein Energy Landscape Exploration) software provided several binding-energy optima for anthraquinone-type Reactive Blue 19 near the aromatic residues and the heam access channel. Subsequent QM/MM calculations showed a higher tendency of TrP-377 than other exposed heam-neighbouring residues to harbour a catalytic protein radical. The existence of such radical was shown by low temperature EPR on the H₂O₂-activated DyP, being identified a mixed tryptophanyl/tyrosyl radical with a multifrequency EPR approach. The signal was dominated TrP-377 neutral radical contribution bv which



Heme prosthetic group (gray), Trp (green), and Tyr (red) residues in AauDyP (4W7J pdb code).

disappeared in the W377S variant and included a tyrosyl contribution assigned to Tyr-337 after analysing the W377S spectra.

A pure tryptophanyl radical EPR signal is detected at pH 7 in contrast with the mixed signal observed at pH 3. The presence of a second tyrosine radical 147) is deduced /Tyr by а multifrequency EPR study of a variety of simple and double-directed variants at different freezing times after their activation by H₂O₂. Such results point out that subsidiary long electrontransfer pathways enter into operation when the main pathway is removed by directed mutagenesis, with catalytic efficiencies progressive decreasing. Finally, self-reduction of the Trp377 neutral radical is observed when reaction time (before freezing) is increased in the absence of reducing substrates (from 10 to 60 s). Interestingly, the tryptophanyl radical is stable in the Y147S/Y337S variant, indicating that these two tyrosine residues are involved in the selfreduction reaction.



EPR spectra of WT DyP and its W377S variant(A) Xband EPR spectra of WT DyP at pH 3 before (top) and after (bottom) the addition of H_2O_2 (and rapid freezing). (**B** and **C**) Narrow scan X-band (v =9.39 GHz) and W-band (v =94.29 GHz) respectively of the radical species. The positions of the three g-tensor components of the tyrosyl contribution are indicated. (**D**) X-band EPR spectrum of the radical intermediate formed in the W377S variant paired with its better simulation (Sim).

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2C – Biotechnological applications of oxidases

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Aims

Different oxidases (versatile peroxidase, dye peroxidase, laccase) are understudy for biotechnological applications in the presence of different substrates like lignin polymer and its derivatives, industrial dyes in order to test their double functions: depolymerisation and synthesis of new materials.

Results

Versatile peroxidase (VP) is a high redox-potential peroxidase of biotechnological interest that is able to oxidize phenolic and non-penolic aromatics, Mn(II) and different dyes. The ability of VP from Pleurotus eryngi to oxidize water soluble lignins (softwood and hardwood lignosulfonates) was demonstrated by the combination of directed mutagenesis and spectroscopic techniques. In addition direct electron transfer between the peroxidase and the lignin macromolecules was kinetically characterised using stopped-flow spectrophotometry. VP variants were used to show that the reaction strongly depends on the presence of the solvent-exposed tryptophan residue (Trp164). Moreover, the tryptophanyl radical detected by EPR spectroscopy of H_2O_2 -activated VP (being absent from the W164S variant) was identified as catalytically active because it was reduced during lignosulfonate oxidation, resulting in the appearance of a lignin radical. Size-exclusion chromatography showed an increase of the molecular mass of the modified residual lignin, especially for the (low molecular mass) hardwood lignosulfonate, revealing that the oxidation products tend to recondense during the VP treatment.



Environment of the exposed catalytic tryptophan acting as starting point for LRET to heme in VP.



EPR spectra of the reactions of VP with H_2O_2 (at molar ratio 1:8), and of VP with H_2O_2 and softwood lignosulfonate at two different molar ratios (1:8:4 or 1:8:12).

The mechanisms of industrial dye transformation by versatile peroxidase from Bjerkandera adusta were elucidated. The EPR analysis on two copper-containing dyes, reactive violet 5 (azo) and reactive blue 72 (phthalocyanine) after enzymatic decolorization showed the cleavage of the azo bond in azo dyes and the total disruption of phthalocyaninic ring in the phthalocyanine dyes. The role of the catalytic Trp172 in the dye transformation by long-range electron transfer pathway was confirmed and also an oxidation mechanism was proposed.

Furthermore the catalytic properties of a VP from Bjerkandera adusta through the chemical modification of the protein surface with free-radical forming Trp residues has been investigated and a new high redox potential laccase POXA1b from Pleurotus ostreatus and its variant have been produced and characterised spectroscopically. Thanks to their characteristics (chemical derivatization and high redox potential) both these last systems seem to be good candidate for biotechnological applications.

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2C – A comparative study of chromatographic matrices for affinity chromatography of CRM197

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Aims

In this study we showed a comparison of three matrices suitable for the purification and refolding of recombinant CRM197 by metal chelating affinity chromatography.

Results

The CRM197 protein is a variant of the diphtheria toxin (DTx, 58 kDa) characterized by a single mutation that reduces its toxicity, (i.e. a glycine-glutamic acid substitution in position 52). Our previous studies indicated the possibility to overexpress the protein in Escherichia coli by using an artificial sequence associated with a short oligonucleotide encoding a hexa-histidine tag. Accordingly, a metal chelating affinity chromatography (IMAC) was used for its purification. We firstly used a standard matrix consisting of agarose beads (HiTrap Chelating Sepharose HP, GE Healthcare Life Sciences) and we always found a higher recovery of CRM197his under denaturing than under refolding conditions. We decided to compare this standard matrix with two different commercial matrices, a macroporous silica matrix (Protino Ni-IDA, Macherey-Nagel) and the synthetic Profinity IMAC resin based on polymeric UNOsphere beads (Bio-Rad). The same extraction procedure, identical quantity of bacterial cultures (300 mL) and comparable amount of protein (from 32 to 37 mg) were used to compare the matrices. Firstly, the purification was performed under denaturing conditions using 6 M urea. Table 1 reported the binding capacity and the recovery for each matrix. The agarose-based matrix seems to bind all proteins loaded on the column but the elution profile was broad and diluted along the elution gradient. The maximum protein recovery was 43-44 %. Contrarily, the silica and polymeric matrices showed a narrower elution profile with a comparable recovery yield of 54-55 % and the recombinant protein was eluted in a small volume of buffer (7-8 mL) with a final concentration of 2.3-2.4 mg/mL.

Table 1. Affinity chromatography of CRM197his under denaturing conditions

Matrix	Input (mg)	Flow through (mg)	Elution (mg	Elution (mL)	Recovery (%)
HiTrap Chelating Sepharose	37	-	16.2	28	44
Protino Ni-IDA	32	8.5	17.2	8	54
Profinity IMAC	33.3	6.9	18.3	7	55

Afterwards, we compared the efficiency of the on-column refolding process using the same three matrices. After loading the sample and washing the column, the urea was removed by two inverse gradients (from 6 to 2 M and from 2 to 0 M urea in 50 mM Tris-HCl pH 7.5, 500 mM NaCl, 1% Triton X-100) before the elution with a linear gradient of imidazole. Preliminary assays with the agarose-based resin showed a very

low yield of recovery (never more than 10 %). When we used the Profinity polymeric matrix, the initial refolding yield was low (13 %), and a high amount of CRM197his was lost inside the flow through during the loading step (Fig. 1(A)(C)). However, when the protein sample was loaded onto the column and the flow-through was reloaded (1 cycle, B), the final recovery increased to 31%, yielding to 9-10 mg of renaturated protein (about 30-32 mg/L). Moreover, as visible in SDS-PAGE (Fig. 1(D)), the band related to CRM197his was detectable in only 5-6 eluted fractions containing 300-340 mM imidazole.



Fig. 1: Purification and refolding of CRM197his by using the Profinity IMAC resin. Chromatographic profiles of the refolding process without (A) or with (B) reloading the flow-through onto the column. (C), (D) SDS-PAGE analysis related to process (A) and (B).

Finally, in order to verify the correct refolding of CRM197his purified with the Profinity IMAC matrix (with recycle), we performed a DNase assay based on agarose gel electrophoresis (data not shown). We found that the on-column refolding procedure allows the recombinant protein to be properly refolded and active.

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2C – Enzyme-containing paints inhibit the growth of marine microorganisms

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Aims

A new strategy to prevent the biofouling of water-submerged surfaces is presented here. In particular, we show that carbonic anhydrase from *Methanosarcina thermophila* can be entrapped into polyacrylic paints.

Results

In conventional practice, paints containing antimicrobial chemicals, e.g. copper, Zinc pyrithion, chlorothalonil, or Sea-Nine are used to delay the fouling of watersubmerged surfaces. However, considering the environmental impact of traditional antimicrobials, alternative antifouling strategies were recently considered. Interestingly, enzyme-containing paints were patented as antifouling agents and, recently, encapsulated enzymes were used to prevent biofouling. A major problem concerning the addition of enzymes to antifouling paints is the presence of organic solvents, whose use generally inactivates the enzymes.

Here we present a radically new, acting at a distance, antifouling strategy, i.e. the physical inhibition of microbial colonization of water-submerged surfaces. We show here that the CO_2 released by paint-entrapped carbonic anhydrase is an effective mean to prevent the fouling of water-submerged surfaces. The use of carbonic anhydrase seems ideal to water environments, due to the natural presence of carbonated salts, leading to the production of CO_2 , preventing biofouling. Further, CO_2 can feature biocide effects on the fouling organisms present on the water-submerged surface of manufactures, but is devoid of eco-toxicological effect.

First, we investigated the overexpression levels of Methanosarcina thermophila carbonic anhydrase (Cam) in Escherichia coli (data not shown). Therefore we decided to evaluate the stability of Cam at 54 °C. Surprisingly, 14 days after the onset of the thermal treatment, Cam did fully retain its initial activity (Figure 1a). The thermal treatment triggered the aggregation and sedimentation of E. coli proteins; therefore, the specific activity of Cam did consistently increase over the time interval considered (Fig. 1b). When we tested the stability at room temperature in seawater, Cam did perform well, retaining about 20 % of its initial activity after 30 days (Fig. 1c). Finally we tested the CO_2 -releasing activity of fiberglass slides (25 cm²) painted with enzymefree or enzyme-containing polystyrene resin (Fig. 1d). To obtain enzyme-containing slides, lyophilized carbonic anhydrase from Methanosarcina thermophila was dissolved into polystyrene resin (Crilat D120S, Vinavil, Milano, Italy), and the paint accordingly prepared was uniformly distributed over fiberglass slides previously treated with an appropriate primer (Marine Primer, Attiva Marine by Bartolomeo Boero, Genova, Italy). Enzyme-free slides were prepared using the same procedure and a polystyrene resin devoid of carbonic anhydrase.



To assay enzyme activity, the slides were half-immersed into a vessel containing 200 mM Tris buffer (pH 7.6). A CO₂-sensitive electrode was then dipped into the vessel, and reactions were started by the addition of 5 mM NaHCO₃.

Remarkably,we detected net CO₂ release from the enzyme-containing slides at a rate equal to $68 \pm 34 \ \mu g/L \cdot s$ (Fig. 1d), corresponding to $1.55 \pm 0.77 \ \mu M/s$.

We indeed reasoned that the release of CO_2 by the paint-entrapped enzyme would physically and chemically inhibit the colonization of water-submerged surfaces by microorganisms. In particular, we expected that a CO_2 -releasing surface would physically (mechanically) hamper the adsorption of microorganisms, whose the growth would be chemically inhibited by the concomitant increase in CO_2 concentration.

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2C – The multifaceted benefits of protein co-expression in *Escherichia coli*

A. Stefan, A. Ceccarelli, E. Conte, A. Montòn-Silva, A. Hochkoeppler

Aims

Here we report on the usefulness of protein co-expression in *Escherichia coli* that is a powerful alternative to the reconstitution *in vitro* of protein complexes, and is of help in performing biochemical and genetic tests *in vivo*.

Results

Two main strategies of protein co-expression in E. coli can be pursued: i) the use of a single plasmid to host the different genes to be overexpressed; ii) the use of multiple plasmids in single cells to co-express the target proteins. This first approach is quite simple, however, the use of a single plasmid to co-express different proteins faces two major difficulties: i) the molecular mass of the vector increases with the number of hosted genes, limiting the number of co-expressed proteins; ii) when multiple genes are cloned under the control of a single promoter, polarity can decrease the expression of the genes distal from the promoter. We recently constructed the pGOOD plasmid compatible to the pBAD vector; in fact, pGOOD features a p15A origin of replication, a tetracycline-resistance cassette and lac-derived regulatory elements. Therefore, coexpression of protein complex is strictly dependent on the addition to the E. coli culture medium of both IPTG and arabinose, triggering overexpression from pGOOD and pBAD, respectively. Interestingly, protein co-expression can efficiently solve difficulties linked to the poor solubility of a protein complex subunit. In addition, in vivo protein complementation tests can be performed, and the protein co-expression can be also use to tune mutation frequency in E. coli. Here we illustrate some examples of each case study by using the pGOOD-pBAD couple.

Example 1: co-expression of α and ε subunits of E. coli DNA polymerase III catalytic core. Cells were grown in the absence of inducers, in the presence of arabinose only, of IPTG only, or in medium supplemented with both arabinose and IPTG (lane 1-4):



Example 2: co-expression can also be used to perform inter-species complementation tests. To evaluate the competence of *Deinococcus radiodurans* polymerase III α subunit (αDr) in binding *E. coli* ε subunit, we have cloned into the pBAD vector a synthetic gene coding for αDr and we have co-transformed *E. coli* with pBAD- αDr and pGOOD- ε . Figure A shows the SDS-PAGE of total protein extracts isolated from cells not induced (lane 1), or induced to overexpress αDr , ε , or αDr and ε (lanes 2-4, respectively). A gel filtration column, loaded with soluble proteins, was used to evaluate complex formation (B, chromatogram empty circles).



Example 3: co-expression of the wild-type and mutagenic ε subunit of *E. coli* DNA polymerase III allows to tune the mutation frequency of the bacterial host. Mutator strains, featuring mutation frequencies higher than their wild type counterparts, are of interest in biotechnology. Protein co-expression can be used to obtain a better control of mutator strains. To this aim, we co-transformed *E. coli* with pBAD- ε and pGOOD1- ε D12A, in order to induce the expression of the wild-type and the mutagenic D12A variant of ε with arabinose and IPTG, respectively. As a phenotypic test, we determined the appearance of β -glucosidase activity, which is cryptic in wild-type *E. coli*. When cells were induced to express the D12A mutagenic variant, β -glucosidase activity was acquired in ca. 20 generations (data not shown).

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2C – Oleuropein degradation by olive leaf protein extract

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Aims

Use of olive leaves as low cost source of substances for interesting biotechnological application.

Results

The enzymatic activity of raw protein olive leaf extract has been investigated in vivo, on olive leaf homogenate and, in vitro with pure oleuropein and other phenolic substrates. At least two types of enzymes were found to be involved in the degradation of endogenous oleuropein in olive leaves. As for the in vitro experiments, the presence of active polyphenoloxidase and β -glucosidase was determined by HPLC and UV–Visible spectroscopy. Interestingly, both the enzymatic activities were found to change during the storage of olive leaves. Specifically, the protein extracts obtained from fresh leaves showed the presence of both the enzymatic activities, because oleuropein depletion occurred simultaneously with the formation of the oleuropein aglycon, 3,4-DHPEA-EA. In comparison leaves subjected to the drying process showed a polyphenoloxidase activity leading exclusively to the formation of oxidation products responsible for the typical brown coloration of the reaction solution.



Fig. 1: Representation of the olive leaves protein extract (left) and HPLC chromatograph of the oleuropein hydrolysis within 5 hours (right).

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Fig. 2: Oleuropein hydrolysis and 3,4-DHPEA-EA formation produced by raw protein extract from fresh olive leaves at 60°C.Concentrations were measured by HPLC analyses.

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2C - Thermodynamics Properties and Photodegradation Kinetics of Indocyanine green in aqueous solution

F. Di Nezza, G. Guerra, C. Costagliola, L. Zeppa, L. Ambrosone

Aims

Indocyanine green (ICG) was approved by the Food and Drug Administration as an agent to evaluate hepatic function, cardiac output and for ophthalmic angiography. ICG has to be administrated in the form of aqueous solutions. However, in aqueous solutions ICG undergoes trans- formations as aggregations and degradation. Such changes result in discoloration decreased light absorption, decreased fluorescence and a shift in the wavelength of maximum absorption. The purpose of the paper is to obtain chemical and physical information about ICG in order to design with less risk possible canalostomy intervention. Therefore the degradation kinetics of the dye when the solution is irradiated with white light has also been studied.

Results

Recently we proved that an aqueous solution of ICG, comprising viscoelastic chondroitin sulfate and sodium hyaluronate, is an effective contrast medium in viscocanalostomy interventation. In this paper our research is focused on dye-dye attractive forces which are generated in aqueous solutions. In aqueous solution of ICG solute-solute interactions, which induce the formation of molecular aggregates such as dimers or n-mers, are highly favored. The fluorescence intensity as a function of the



arc strategy is employed to evaluate the evolution speed of the degree of conversion. The method does not provide information about the molecular mechanism, but the lifetime and the apparent reaction order of overall kinetics is fully determined. We are confident that the equations obtained can be of any practical use in planning surgery for glaucoma. dye concentration shows a maximum. Spectrophotometric results indicate that the dimerization reaction rapidly reaches equilibrium. A new approach was used to calculate the equilibrium constant for the dimerization reaction. The value obtained is comparable to those obtained with different methods on safranine and thionine. ICG white light degrades. The exposed to degradation kinetics is monitored spectrophotometrically and results interpreted on the basis of a direct model. The moving



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2C – In Vivo Near-Infrared Fluorescence Imaging of Aqueous Humor Outflow Structures

L. Zeppa, L. Ambrosone, G. Guerra, M. Fortunato, C. Costagliola

Aims

The aim of this study has been to visualize the aqueous out how system in patients a ected by primary open angle glaucoma. A solution of indocyanine green (ICG) plus high viscosity viscoelastic solution was injected into the Schlemm canal (SC) during surgery in 10 glaucomatous patients undergoing canaloplasty.

Results

Soon a er injection of the dye, there was impregnation of the borders of the scleral ap due to partial re ux caused by the intrachannel resistance; progression of the dye along

the SC starting from the site of injection was then visualized. In some eyes, the filling proceeded along 360 degrees whereas in others only a portion of the canal was visualized. In 3 patients, the percentage of lling was 70%, whereas in the 7 patients this remaining percentage decreased up to 50%. A correlation between SC lling and number of CCs visualized was observed. It is possible that an obstruction of the canal was present in such



eyes. e lling of the collector channels occurred only in correspondence of the patent



portions of the SC. However, even in presence of a patent SC over 360 degrees, the filling of the collector channels was not simultaneously visualized in all four quadrants. Furthermore, the collector CCs closer to the site of injection did not necessarily ll up before the farther ones.



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2C – Physico-Chemical Properties of Pharmaceutical Systems

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Aims

The research activity in the pharmaceutical field concerns the development of methods for the resolution of problems related to the preformulation phase of active principles. The topics of interest are: polymorphism and stability of drugs in the solid state, host-guest systems, drug-excipient compatibility, crystallinity degree and phase diagrams characterization, strategies to improve the solubility and the dissolution rate of drugs. In particular, in the years 2014-2016 the efforts have been directed towards the preparation and the characterization of co-crystals and of electrospun fibers to enhance or to control the drug release.

Results

Solubility represents an important challenge for formulation of drugs, because the therapeutic efficacy of a drug depends on the bioavailability and ultimately on its solubility. Low aqueous solubility is one of the main issues related with formulation design and development of new molecules. Many drug molecules present bioavailability problems due to their poor solubility. For this reason there is a great interest in the development of new systems able to enhance the dissolution of poorly water-soluble drugs.

We prepared co-crystals of bumetanide, a diuretic and natriuretic active principle, with 4-amino benzoic acid. The synthesis was performed both by wet and dry grinding. The co-crystal formation was investigated with a wide range of techniques, including solid-state NMR, IR, XRD, microscopy and thermal analysis. Wet and dry grinding procedures led to different co-crystal polymorphs. In particular, the dry method gave a co-crystal by powder amorphization and subsequent crystallization. DFT calculations at B3LYP/6-31+G(d,p) level of theory shed light on the H-bond scheme at the basis of co-crystals formation. Both the co-crystals showed improved solubility and dissolution rate with respect to the drug alone. This could guarantee a faster absorption and a better bioavailability of the active principle.

Electrospun fibers loaded with budesonide have been fabricated and characterized with the aim of controlling the drug release in the gastrointestinal tract. Budesonide is a non halogenated glucocorticosteroid drug, highly effective in the treatment of some inflammatory bowel diseases with local action throughout ileum and colon. At this aim, Eudragit® S 100, a polymer soluble at pH>7, commonly used for enteric release of drugs, has been successfully spun into ultrafine fibers loaded with budesonide at 9% and 20 % (w/w) using the electrospinning process. The physico-chemical characterization by scanning electron microscopy, X-ray diffraction, FT-IR spectroscopy and thermal analyses indicated the amorphous nature of budesonide in the electrospun systems. Dissolution rate measurements using a pH-change method showed negligible drug dissolved at pH 1.0 and sustained release at pH 7.2. Therefore, the pharmaceutical systems proposed, made of fibers, represent an effective method for drug targeting to terminal ileum and colon with the aim of improving the local efficacy of this drug.

We prepared fibers containing perphenazine, an insoluble model drug, by the electrospinning method, in order to increase its water solubility. Two hydrophilic polymers, polyvinylpyrrolidone (Plasdone® K29/32) and polyvinyl caprolactam-polyvinyl acetate-polyethylene glycol graft copolymer (Soluplus®) were used.

The physico-chemical characterization suggests that the drug loaded in the fibers is in the amorphous state. Both polymeric carriers are effective to promote the drug dissolution rate in water, where this active is insoluble, due to the fine dispersion of the active into the polymeric matrices, obtained with this production technique. In fact, the dissolution profiles of the fibers, compared to the simple physical mixture of the two components, and to the reference commercial product Trilafon® 8 mg tablets, show that a strong enhancement of the drug dissolution rate can be achieved with the electrospinning technique.

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2C – Phospholamban (PLN) regulation of sarco/endoplasmic reticulum Ca-ATPase (SERCA)

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Aims

Investigation of the interaction mechanism between Phospholamban (PLN) and sarco/endoplasmic reticulum Ca-ATPase (SERCA).

Results

SERCA promotes muscle relaxation by pumping Ca^{2+} ions from the cytoplasm into the sarcoplasmic reticulum lumen. The activity of SERCA in cardiomyocytes is regulated by a small membrane protein, PLN. It is known that PLN exists as a monomer and homopentamer, both of which are critical for normal cardiac function and can interact with SERCA. Previous studies have shown that recombinant wildtype PLN can form a cation selective ion channel in different biomimetic membranes [1–4].

In the present study we evaluated the effects of PLN on the ATP-dependent Ca^{2+} translocation by SERCA by performing pre-steady state current measurements on a solid supported membrane (SSM, Figure 1A). Proteoliposomes incorporating SERCA and PLN were adsorbed on a SSM and then activated by ATP concentration jumps. The charge obtained by numerical integration of the ATP-induced current transient is attributed to an electrogenic event corresponding to the translocation and release of bound Ca^{2+} upon ATP phosphorylation within the first enzyme cycle [5].

Our results indicate that PLN interferes with ATP-dependent Ca^{2+} translocation by SERCA. By fitting the translocated charges at various Ca^{2+} concentrations using the Hill function, we compared the K_{0.5} and cooperativity coefficient values (Figure 1B). A higher K_{0.5} value was observed in the presence of PLN with respect to the value determined for proteoliposomes containing SERCA only. This result suggests that PLN decreases SERCA calcium affinity. Moreover, in the case of co-reconstituted SERCA/PLN proteoliposomes high K_{0.5} and cooperativity values were obtained with simultaneous ATP and Ca²⁺ concentration jumps, while a much higher K_{0.5} and loss of cooperativity were observed with Ca²⁺ jumps in the presence of ATP.

Therefore, SERCA inhibition by PLN occurred under different substrate conditions. The choice of substrate conditions is important to promote particular conformational states of SERCA. Overall, our observations support the concept that PLN can establish an inhibitory interaction with at least two SERCA conformational states, thereby decreasing the calcium affinity of the enzyme.



Fig. 1A: SSM technique. Schematic diagram of a proteoliposome incorporating SERCA and PLN adsorbed to a SSM and subjected to an ATP concentration jump.

Fig. 1B: Co-reconstituted SERCA and PLN proteoliposomes activated by ATP and Ca^{2+} concentration jumps. Normalized charges related to simultaneous ATP (100 μ M) and free Ca^{2+} (various concentrations) jumps (circles; blue line). Normalized charges related to free Ca^{2+} (at different concentrations) jumps in the presence of 100 μ M ATP (triangles; black line). Normalized charges related to ATP concentration jumps on proteoliposomes containing SERCA+PLN in the presence of different Ca^{2+} concentrations (squares; red line). The lines represent curve fitting of the experimental data using the Hill equation. Error bars represent SEM of at least four independent measurements.

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2C – Interaction of antitumor drugs with P-type ATPases

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Aims

Mechanism of interaction of antitumor compounds with P-type ATPases. Role of P-type ATPases in anticancer treatment.

Results

P-type ATPases are a large and varied family of membrane transporters that couple the energy provided by ATP hydrolysis to the active transport of various ions across biological membranes. A specific feature of P-type ATPases is the formation of a phosphorylated intermediate state during their catalytic cycle.

The ion transport mechanism of P-type ATPases has been investigated by electrophysiological measurements on solid supported membranes (SSM) [1]. The SSM consists of a hybrid alkanethiol/phospholipid bilayer supported by a gold electrode. Proteoliposomes or native membranes (vesicles or fragments) incorporating the ATPase can be adsorbed on a SSM and activated by a rapid substrate concentration jump. The substrate jump induces charge movement across the transport protein, and a current transient can be detected by the SSM method [1].

We evaluated the inhibitory effects of the antitumor drug cisplatin on the pumping activity of sarcoplasmic reticulum (SR) Ca^{2+} -ATPase and Na^+,K^+ -ATPase by employing the SSM-based electrophysiological method. We performed ATP concentration jumps in the absence (control measurement) or in the presence of cisplatin and recorded the relative current signals.

In the case of SR Ca²⁺-ATPase, we found that cisplatin strongly interferes with translocation of Ca²⁺ ions upon ATP phosphorylation (Fig. 1). We evaluated the concentration dependence of the cisplatin inhibitory effect and we found an IC₅₀ value of 1.3µM, indicating that cisplatin acts as a high affinity Ca²⁺-ATPase inhibitor. It is worth mentioning that an IC₅₀ value of ~ 1µM was also reported for the anticancer ruthenium (III) complex KP1019, which was found to affect ATP-dependent calcium translocation by SR Ca²⁺-ATPase [2].

We also observed an inhibitory effect of cisplatin on the pumping activity of Na⁺,K⁺-ATPase (Fig. 2). However, in the case of Na⁺,K⁺-ATPase inhibition by cisplatin an IC₅₀ value of 11µM was found, suggesting that cisplatin acts as a less potent inhibitor towards Na⁺,K⁺-ATPase as compared to SR Ca²⁺-ATPase.



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Fig. 1: Effect of cisplatin on SR Ca²⁺-ATPase. Current transients induced by ATP concentration jumps in the absence (control measurement, black line) or in the presence of 5μ M cisplatin (red line). Inset: Normalized charges in the absence or in the presence of cisplatin (2μ M and 10μ M). The error bars represent S.E. of three independent measurements.



Fig. 2: Effect of cisplatin on Na⁺,K⁺-ATPase. Current transients induced by ATP concentration jumps in the absence (control measurement, black line) or in the presence of 5μ M cisplatin (red line). Inset: Normalized charges in the absence or in the presence of cisplatin (5μ M and 20μ M). The error bars represent S.E. of three independent measurements.

Recently, the SSM technique was employed to investigate Cu^+ ion movement in bacterial (*LpCopA*) [3] and human Cu^+ -ATPases (*ATP7A* and *ATP7B*) [4]. In particular, we demonstrated that cisplatin and oxaliplatin can activate ATP7A and ATP7B, whose normal function is to catalyze active transport of Cu^+ across cellular membranes, and undergo ATP-dependent translocation in a fashion similar to that of Cu^+ [5]. We also found that the Pt-related charge movement is dependent on formation of a phosphorylated intermediate, as well as conformational adjustments analogous to those required for Cu-related charge translocation.

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2C – Glutathione, glutathione disulfide and S-glutathionylated proteins in cell cultures

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Aims

To develop and validate a new protocol to measure glutathione (GSH), glutathione disulfide (GSSG) and S-glutationylated proteins (PSSG) in a large series of cell lines.

Results

We demonstrate that the major artifact occurring during thiol and disulfide analysis in cultured cells is represented by glutathione disulfide (GSSG) and S-glutathionylated proteins (PSSG) overestimation due to artificial oxidation of glutathione (GSH) during sample manipulation, and that this methodological problem can be solved by the addition of N-ethylmaleimide (NEM) immediately after culture medium removal. Basal levels of GSSG and PSSG in different lines of cultured cells were 3-5 and 10-20 folds higher, respectively, when the cells were processed without NEM. NEM pretreatment prevented also the artificial reduction of disulfides that occurs during the pre-analytical phase when cells are exposed to an oxidant stimulus. In fact, in the absence of NEM, after medium removal, GSH, GSSG and PSSG levels restored their initial values within 15-30 min, due to the activity of reductases and the lack of the oxidant. The new developed protocol was used to measure the thiol-disulfide redox status in 16 different line cells routinely used for biomedical research both under basal conditions and after treatment with disulfiram, a thiol-specific oxidant (0-200 µM concentration range). Disulfiram (Antabuse®) is a drug used to treat chronic alcoholism since it induces an extremely adverse reaction when taken in the presence of alcohol by inhibition of acetaldehyde dehydrogenase and is currently being studied as a treatment for cocaine dependence, for its antiprotozoal activity, in cancer therapy and as a treatment in HIV. It possesses a reactive disulfide bond, which reacts readily with both protein and low-molecular mass thiols forming mixed disulfides, disulfides and dithiocarbamates.





Study of the protective effect of NEM. BAEC were treated (black bars) or not (gray bars) with 5 mM NEM. Cells were then lysed by TCA addition and analyzed for the content of GSH, GSSG and PSSG by HPLC. **p<0.01 vs NEM treatment. Data are the mean \pm SD, n = 3.

Our data indicate that in most cell lines, treatment with disulfiram affected the levels of GSH and GSSG only at the highest concentration. On the other hand, PSSG levels increased significantly also at the lower concentrations of the drug and the rise was remarkable (from 100 to 1000 folds at 200 μ M concentration) and dose-dependent for almost all the cell lines. These data support the suitability of the analysis of PSSG in cultured cells as a biomarker of oxidative stress.

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2C – Graphene/Nanoparticles hybrid system for the controlled immobilization of biomarkers for early diagnosis of neurodegenerative diseases

C. Lofrumento, M.R. Martina, G. Caminati

Aims

Aim of the research project is the design and fabrication of novel hybrid nanostructures as diagnostic platforms for the determination of biomarkers for the very early stage of neurodegenerations, such as Alzheimer's disease.

The nanostructures result from a combination of ordered and compact arrays of metal nanoparticles veiled with graphene derivatives. The external layer is functionalized with proper receptors of the selected biomarker, immobilized with the fine tuning of its surface density and molecular conformation on the sensor transducer.

Results

We fabricated monolayer assemblies of silver nanocubes (AgNCs), by means of the Langmuir-Blodgett (LB) technique, as a convenient nanostructural basal layer upon which, one-atom-thick GO sheets with lateral dimensions of few microns were deposited. The adsorption process was followed by a Quartz Crystal Microbalance (QCM) with dissipation monitoring that provided mass-density, thickness and elasticity values for the GO layer at saturation. A sketch of the resulting structures is reported in figure 1.



Fig. 1: Cartoon of the proposed sensors platform and Atomic Force Microscopy image of the system

The novel nanostructure was used for the detection of fibrillated lysozyme, as model biomarker for amyloid diseases. The adsorption of native and fibrillated lysozyme on the nanosensors was investigated as a function of bulk protein concentration with a variety of techniques: QCM, Confocal Laser Scanning Microscopy and Atomic Force Microscopy to obtain the surface density and thickness of the lysozyme. CLSM allowed to visualize the morphology of the aggregated fibrils whereas spatially resolved fluorescence spectra of Thioflavine T and Congo Red, used as fluorescence probes for the β -sheet structure, allowed to correlate the morphology of the fibrils with the secondary structure of the protein. Finally, we performed Surface Enhanced Raman Spectroscopy (SERS) analysis on the same samples for the identification of specific signals of secondary structure of native and fibrilled lysozyme (figure 2).



Fig. 2: (a) Lysozyme fibrils observed by CLSM and (b) SERS spectra of globular lysozyme (red line) and fibrillar lysozyme (black line)

The proposed nano-platform represents a valuable substrate for the accurate differentiation between the globular and the fibrillar structures of lysozyme. QCM results combined with SERS analysis allowed for the determination of subnamolar concentration of Lysozyme and to discriminate between the toxic and native form of the protein.

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