

Workshop

Advanced inorganic materials: green and unconventional synthesis approaches and functional assessment

**Department of Chemical Sciences
University of Padova
Padova, September 5-7th, 2018**

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Ms. Lucia Zanetti (DiSC)

Keynote Speakers (alphabetic order)

1. **Prof. Jaakko Akola**, Tampere University of Technology, Finland
"Computational design of transition metal nanocluster catalysts for (electro)chemical reactions involving hydrogen"
2. **Prof. Lourdes Calzada**, Instituto de Ciencia de Materiales de Madrid, Spain
"Low-temperature crystallization of solution derived metal oxide thin films assisted by chemical processes"
3. **Prof. Paolo Fornasiero**, University of Trieste, Italy
"Sustainable synthesis methods of smart nanocatalysts?"
4. **Prof. Michael Fröba**, University of Hamburg, Germany
"Templated synthesis of nanoporous materials in different morphologies"
5. **Dr Patricia Hernandez-Fernandez**, Danish Technological Institute, Denmark
"Up-scaling the production of functional nanomaterials with tailored properties using continuous supercritical flow synthesis"
6. **Prof. Katharina Landfester**, Max Planck Institute for Polymer Research, Germany
"Miniemulsions as nanoreactors for the synthesis of inorganic nanomaterials for bio-applications and catalysis"
7. **Prof. Sebastian Polarz**, University of Konstanz, Germany
"Shape and 'impurities' of nanomaterials as a tool to control functional properties"
8. **Prof. Bernd Smarsly**, Justus-Liebig-University Gießen, Germany
"Ionic liquids for the low T synthesis of inorganic nanocrystalline materials"
9. **Prof. Richard Walton**, University of Warwick, United Kingdom
"Watching solids crystallise and react using in situ analytical methods"

Prof. Jaakko Akola (Norwegian University of Science and Technology -NTNU)

Prof. Jaakko Akola is full professor in Computational Physics since 2017 in the Department of Physics, Norwegian University of Science and Technology (NTNU). He is also affiliated with the Tampere University of Technology, Finland, where he worked as a group leader and associate professor (tenure-track) during 2010-2016. Until 2017, his group was also part of the Finnish Centre of Excellence in Computational Nanoscience in the Aalto University.

Prof. Akola is a specialist in atomistic simulations using DFT, classical molecular dynamics, and Monte Carlo methods, and in particular he has concentrated on atomistic/electronic properties of nanoparticles, interfaces, and amorphous/glassy materials. Currently, computational catalysis research is one of his main research themes, and his group works on DFT simulations and ideas based on machine-learning to develop more efficient tools for atomistic simulations and materials screening. Prof. Akola is the coordinator of the H2020-NMP project “CritCat” (2016-2019) on rational design of future catalyst materials for hydrogen energy, and he leads the ALLDESIGN project (NTNU Digital Transformation, 2019-2022) on multiscale modelling and design of aluminum alloys. His publication record comprises over 100 articles, including publications in Science, Nature series, PNAS, Nano Letters, etc. with > 5000 citations (h-index 30). Prof. Akola has a vast international network based on his experience as a project coordinator, leading editorial role in a scientific journal (Advances in Physics: X), proposal reviewer (e.g. FP7, H2020, ERC), and several extended research periods/visits abroad (Germany, Japan, Taiwan, USA).

Prof. Maria Lourdes Calzada, Instituto de Ciencia de Materiales de Madrid, Spain

M. Lourdes Calzada is Research Professor of the Spanish National Research Council (CSIC, Spain), at the Materials Science Institute of Madrid (ICMM). Here, she leads the

research line on “*Functional metal oxide thin films*”. Key points of this investigation are the “*Development of low-temperature sol-gel synthesis strategies to attain metal oxide materials*” and the “*Integration of functional films and self-assembled systems with semiconductor and flexible substrates (Si-technology and Flexible Electronics)*”. In the framework of this area, her group is pioneer in the “*Low-temperature solution processing of ferroelectric and multiferroic complex oxides for flexible electronic devices*”.

Prof. Calzada has been Principal Investigator of several National and European projects and has published more than 180 publications. She has presented more than 10 invited talks in International Conferences, has published 10 book chapters and is co-inventor in 3 patents of application. She has supervised 6 PhD theses, two of them PhD extraordinary awards in chemistry, and several M.Sc Thesis. She belongs to the steering committees of several National and International Conferences and participates in university under- and post-graduate programmes.

Prof. Paolo Fornasiero, University of Trieste, Italy



Paolo Fornasiero obtained his degree in Chemistry in 1992 and his PhD in 1997 at the University of Trieste (Italy). After a post-doctoral fellowship at the University of Reading (UK), he was appointed as an assistant professor in 1998, associate professor of inorganic chemistry in 2006, and full professor in 2016 at the University of Trieste.

His research focuses on the application of inorganic chemistry to nanoscience for the preparation of new materials useful in the fields of energy and environmental protection. He received the 2005 Nasini Gold Medal from the Italian Chemical Society, the 2013 Chiusoli Gold Medal from the Italian Chemical Society, the 2017 Heinz Heinemann Award from the International Association of Catalysis Societies, the 2017 Kramer Award from Istituto Lombardo and the 2018 "Maria Teresa Messori Roncaglia ed Eugenio Mari" prize from Accademia Nazionale dei Lincei.

Prof. Michael Fröba, University of Hamburg, Germany



Michael Fröba studied chemistry in Würzburg and Hamburg and received his doctorate in 1993 from the Institute of Physical Chemistry, where he worked with Prof. W. Metz on graphite intercalation compounds. From 1994 to 1996, he was a Feodor Lynen research fellow in the group of Dr J. Wong at the Lawrence Livermore National Laboratory. After his habilitation at the University of Hamburg in 2000, he was appointed as an Associate Professor for Inorganic Chemistry at the University of Erlangen-Nuremberg. From 2001 to 2007 he was Full Professor for Inorganic Chemistry at the Justus Liebig University of Giessen, and since 2007 he holds a Chair for Inorganic Chemistry at the University of Hamburg. His research has a strong focus on the synthesis, characterization and application of nanoporous (hybrid) materials, with an emphasis on their usage in sorption, electrochemical and thermal energy storage as well as on the investigation of confinement effects and their impact on the properties of intrapore water and aqueous salt solutions.

Dr Patricia Hernandez-Fernandez, Danish Technological Institute, Denmark



Patricia Hernandez-Fernandez (León, Spain, 1980) got a degree in Chemical engineering at the Rey Juan Carlos University of Madrid in 2004. After that, she was awarded the FPI fellowship by the Ministry of Education and Science of Spain to complete a PhD at the Autonomous University of Madrid (UAM), where she got a master degree in Electrochemistry in 2007 and a PhD in Sciences in 2010 (European mention, *cum laude*). She conducted her research at the Department of Applied Physical Chemistry (UAM) and at the Institute of Catalysis and Petrochemistry (CSIC). Her work was focused on the synthesis and characterization of nanoparticulate catalysts for fuel cells. She completed her education with stays at Cornell University (USA) and Université de Poitiers (France) where she learnt about *in situ* characterization techniques. After a postdoc at the University of

Aberdeen (UK), she became Assistant Professor at Autonomous University of Madrid. In 2011 she moved to Denmark to work as a postdoc at the Technical University of Denmark (DTU, Physics department). The main focus of her research was to understand the reasons behind the kinetic improvement that some nanomaterials showed in specific electrochemical reactions. For that purpose, she worked in close collaboration with DFT scientists and specialists in Synchrotron measurements at Stanford University (USA). Since 2013, she is a Senior Specialist at the Department of Nano Production and Micro Analysis at the Danish Technological Institute (DTI). She works with the synthesis of nanomaterials with supercritical flow reactors both in a laboratory scale but also in a pilot scale. Her focus is the optimization of this methodology to fabricate active and stable materials, and the ultimate goal is the up-scaling of this technology to a commercial level. Some of the catalytic applications she is currently studying are fuel cells, electrolyzers, diesel oxidation and three-way catalysts. Patricia Hernández-Fernández has presented her work in around 30 international congresses, delivering 17 oral presentations, 2 keynotes and 17 poster contributions. Her work has resulted in more than 20 scientific papers (*h-index* 16, Scopus 2018) in high impact factor journals (e.g. *Nature Chem.*, *Angew. Chem. Int. Ed.*)

Prof. Katharina Landfester, Max Planck Institute for Polymer Research, Germany



Katharina Landfester received her doctoral degree in Physical Chemistry after working in 1995 at the MPI for Polymer Research (MPIP). After a postdoctoral stay at the Lehigh University (Bethlehem, PA), she worked at the MPI of Colloids and Interfaces in Golm leading the mini-emulsion group. From 2003 to 2008, she was professor at the University of Ulm. She joined the Max Planck Society in 2008 as one of the directors of the MPIP. She was awarded the Reimund Stadler prize of the German Chemical Society and the prize of the Dr. Hermann Schnell Foundation, followed by the Bruno Werdemann Lecturer in 2012 and the Bayer Lecturer in 2014. Her research focusses on creating functional colloids for new material and biomaterial applications.

Prof. Sebastian Polarz, University of Konstanz, Germany



Sebastian Polarz studied chemistry at the University of Bielefeld and received his diploma in 1999 with Prof. A. Müller on polyoxometalate chemistry. He then joined the Max-Planck Institute of Colloids and Interfaces working with Prof. M. Antonietti on confinement effects. After his PhD thesis in 2001, he moved to the group of Prof. G.A. Ozin and conducted research on porous materials. He initiated an Emmy-Noether research group in 2003 in the entourage of Prof. M. Driess first at the Ruhr-University Bochum, then at the Technical University Berlin. Since 2007 he is full professor for 'functional inorganic materials' at the University of Konstanz, and his main research interests are on nanoporous organosilica materials, semiconductor nanostructures and new surfactants.

Prof. Bernd Smarsly, Justus-Liebig-University Gießen, Germany



Bernd Smarsly studied chemistry and physics at the University of Marburg, Germany, and was staying in Innsbruck, Austria, in 1996. He received a Master degree of Natural Sciences in 1998, followed by PhD studies until 2001 at the Max Planck Institute of Colloids and Interfaces, supervised by Prof. M. Antonietti.

In the period 2002–2003 he performed postdoctoral research at the Advanced Materials Laboratory of the University of New Mexico at Albuquerque, USA. From 2003 to 2007 he was working as young research group leader at the MPI of Colloids and Interfaces in the department of Prof. Antonietti. In 2007 he became full professor of physical chemistry at Justus-Liebig University Giessen (Germany). His main research interests functional, mesostructured metal oxides, their physico-chemical properties, and the development of novel characterization techniques, especially using scattering diffraction and scattering techniques.

Prof. Richard Walton, University of Warwick, United Kingdom



Richard Walton was educated at the University of Oxford (BA 1994) and the University of Reading (PhD 1997) and undertook postdoctoral work in the Inorganic Chemistry Laboratory, Oxford with Dermot O'Hare working on *in situ* methods for following crystallisation. Following a Lecturer position at the University of Exeter (2000-2005) he was appointed at the University of Warwick as Senior Lecturer in 2006 and promoted to full Professor of Chemistry in 2011. His research focusses on the synthesis and characterisation (particularly using synchrotron X-rays and neutron scattering) of a range of inorganic materials, including transition-metal oxides, zeolites and MOFs. His work involves several industrial collaborations to examine applications in areas such as heterogeneous catalysis and electrochemistry. He is co-editor (with Bruce and O'Hare) of the *Inorganic Materials Series*, published previously by Wiley and currently the Royal Society of Chemistry, he holds a visiting researcher position at USP Ribeirão Preto (Brazil), and is the holder of a Royal Society Industry Fellowship working with Johnson Matthey plc for 4 years to explore scale-up and new applications the materials produced in Warwick.

AIM 2018 Workshop program

Padova, 5-7th September, 2018



Aula A “Raffaello Nasini”

Department of Chemical Sciences – University of Padova

Via Marzolo, 1 – 35131 Padova

Abbreviations

KN – Keynote lecture (30 minutes + 5 minutes discussion)

OP – Oral presentation (15 minutes + 5 minutes discussion)

FP – Flash presentation (7 minutes + 3 minutes discussion)

05th of September

Opening Session

11:30-12:30	Registration (Aula Studio, via Marzolo)	
12:30-13:30	Lunch Break/Poster Session (Aula Studio, via Marzolo)	
Chairman: Prof. Silvia Gross, Dept. of Chemical Sciences, University of Padova		
13:30-13:45	Opening welcome	<u>Prof. Michele Maggini</u> , Department head, Dept. of Chemical Sciences, University of Padova <u>Prof. Silvia Gross</u> , Dept. of Chemical Sciences, University of Padova
13:45-14:20	KN1	<u>Prof. Lourdes Calzada</u> , Instituto de Ciencia de Materiales de Madrid, Spain "Low-temperature crystallization of solution derived metal oxide thin films assisted by chemical processes"
14:20-14:40	OP1	<u>Dr. Iñigo Bretos</u> , Dept. of Materials for Information Technologies - ICMM-CSIC – Madrid, Spain "A "three-in-one" approach to induce the low-temperature crystallization of BiFeO ₃ thin films"
14:40-15:00	OP2	<u>Dipl.-Ing. Bernd Wittek</u> , UMICORE AG – Hanau, Germany "A sol-gel approach for the production of exhaust catalysts"
15:00-15:20	Coffee break (Aula A, via Marzolo, entrance)	
Chairman: Prof. Jawaad Darr, Materials Chemistry Section - University College London, UK		
15:20-15:55	KN2	<u>Prof. Bernd Smarsly</u> , Justus-Liebig-University Gießen, Germany "Ionic liquids for the low T synthesis of inorganic nanocrystalline materials"
15:55-16:15	OP3	<u>Ms. Karin Rettenmaier</u> , University of Salzburg, Austria "Electrochemical and photochemical deposition of MnO _x on porous ZnO scaffolds"
16:15-16:35	OP4	<u>Dr. Carlos Sotelo-Vazquez</u> , University College London, UK "Continuous hydrothermal flow synthesis of lithium-nickel rich NMC layered materials for lithium-ion batteries"
16:35-18:00	Poster session & Spritz (Aula Studio, via Marzolo)	
18:00-18:10	Gathering for the Social Dinner (Department of Chemical Sciences Entrance, Via Francesco Marzolo 1)	
18:10-18:30	Transfer to the Botanical Garden of Padova	
18:30-19:30	Guided tour of the Botanical Garden (in English or Italian)	
19:30-20:00	Aperitif	
20:30-22:30	Social Dinner (Orto Botanico, Prato della Valle)	

06th of September

Morning Session

Chairman: Dr. Paolo Dolcet, Karlsruhe Institute of Technology, Germany

9:00-9:35	KN3	<u>Prof. Jaakko Akola</u> , Tampere University of Technology, Finland "Computational design of transition metal nanocluster catalysts for (electro)chemical reactions involving hydrogen"
9:35-9:55	OP5	<u>Prof. An Hardy</u> , UHasselt, Institute for materials research IMO-imomec – Diepenbeek, Belgium "The importance of Cu(I) intermediates in self-reducing molecular inks for Cu deposition"
9:55-10:15	OP6	<u>Dr. Maria Chiara Spadaro</u> , Nanomaterials Laboratory - Swansea University, UK "Precise and scalable production of nano-catalysts by nanocluster beam deposition"
10:15-10:35	OP7	<u>Dr. Andrea Vittadini</u> , ICMATE CNR – Padova "Unconventional synthesis of titanium-tetrapyrrole films at TiO ₂ (110): a computational and experimental approach"
10:35-10:55	OP8	<u>Dr. Silvia Carlotto</u> , Dept. of Chemical Sciences - University of Padova "Pigments of life", well-suited molecules to look into the metal:ligand symmetry Restricted covalency"
10:55-11:20	Coffee break (Aula A, via Marzolo, entrance)	
Chairman: Dr. Lucia Curri, IPCF CNR - Bari Division - Dept. of Chemistry - Bari		
11:20-11:55	KN4	<u>Prof. Paolo Fornasiero</u> , University of Trieste "Sustainable synthesis methods of smart nanocatalysts?"
11:55-12:15	OP9	<u>Prof. Siglinda Perathoner</u> , Dept. of Chemical, Pharmaceutical, Biological and Environmental Sciences - University of Messina "Preparation of advanced nanostructured electrodes for energy and chemistry transition"
12:15-12:35	OP10	<u>Prof. Kiyotaka Nakajima</u> , Institute for catalysis - Hokkaido University, Japan "New route for the production of furan 2,5-dicarboxylic acid with a CeO ₂ supported Au catalyst"
12:35-12:55	OP11	<u>Dr. Sara Colussi</u> , Polytechnical Dept. - University of Udine "Solvent-free mechanical synthesis of Pd/CeO ₂ catalysts for methane abatement"
12:55-14:00	Lunch Break (independent)	

Afternoon Session

Chairman: Prof. Michael Fröba, Dept. of Chemistry - University of Hamburg, Germany

14:00-14:35	KN5	<u>Prof. Katharina Landfester</u> , Max Planck Institute for Polymer Research, Germany "Miniemulsions as nanoreactors for the synthesis of inorganic nanomaterials for bio-applications and catalysis"
14:35-14:55	OP12	<u>Dr. Rafael Muñoz-Espí</u> , Institute of Materials Science - ICMUV - Universitat de València, Spain "Colloidal synthetic strategies for the microencapsulation of inorganic phase change materials"
14:55-15:15	OP13	<u>Mr. Fabio Vischio</u> , IPCF CNR - Bari Division - Dept. of Chemistry – Bari "Characterisation of plasmonic copper sulphide nanocrystals containing solid lipid nanoparticles and determination of their concentration"
15:15-15:35	Coffee break (Aula A, via Marzolo, entrance)	
Chairman: Prof. Sebastian Polarz, Dept. of Chemistry - University of Konstanz, Germany		
15:35-16:10	KN 6	<u>Prof. Richard Walton</u> , University of Warwick, UK "Watching solids crystallise and react using in situ analytical methods"
16:10-16:30	OP14	<u>Dr. Gregorio Dal Sasso</u> , IC-CNR - Como "Characterization of N-doped hydroxyapatite nanocrystals through SAXS and synchrotron WAXS Total Scattering Methods"
16:30-16:50	OP15	<u>Dr. Paolo Centomo</u> , Dept. of Chemical Sciences, University of Padova "In-situ/operando investigation of heterogeneous catalysts with XAS"
16:50-17:00	FP1	<u>Mr. Dustin Bauer</u> , University College London, UK "Hydrothermal synthesis of composites of conversion materials and TiO ₂ for Li-ion battery anodes"
17:00-17:10	FP2	<u>Mr. Nicola Dengo</u> , Dept. of Chemical Sciences, University of Padova "Exploring the synthesis of zinc sulfide: design and optimisation of new functional nanostructures"
17:05-17:10	Gathering for the Social Tour (Department of Chemical Sciences Entrance, Via Francesco Marzolo 1)	
17:10-17:30	Transfer to Golena San Massimo	
17:30-18:30	Social Tour "Padova by Boat" & Spritz (Golena San Massimo, Padova)	

07th of September

Morning Session

Chairman: Prof. Bernd Smarsly, Institute of Physical Chemistry - Justus-Liebig-University Giessen - Germany

9:00-9:35	KN7	<u>Prof. Sebastian Polarz</u> , University of Konstanz, Germany "Shape and 'impurities' of nanomaterials as a tool to control functional properties"
9:35-9:55	OP16	<u>Prof. Simone Mascotto</u> , University of Hamburg, Germany "Sustainable fabrication of high temperature SrTiO ₃ -based catalysts"
9:55-10:15	OP17	<u>Prof. Adolfo Speghini</u> , Dept. of Biotechnologies - University of Verona "Luminescent nanomaterials prepared by microwave-assisted hydrothermal synthesis: two interesting cases"
10:15-10:35	OP18	<u>Dr. Maria Cannio</u> , Dept. of Engineering - University of Modena and Reggio Emilia "Facile microwave hydrothermal synthesis of multiferroic micronised particles"
10:35-10:45	FP3	<u>Ms. Chiara DeFilippi</u> , Queen Mary University of London, UK "Sustainable synthesis of readily available metallic ceramics as a new generation of catalyst"
10:45-10:55	FP4	<u>Mr. Enrico Podda</u> , Dept. of Chemical Geological Sciences - University of Cagliari "Ni(II) Square Planar Complexes and 4,4'-Bipyridine based Coordination Polymers by Mechanochemical and Solution-based Synthesis"
10:55-11:25	<u>Coffee break (Aula A, via Marzolo, entrance)</u>	
Chairman: Dr. Rafael Muñoz-Espí, Institute of Materials Science - ICMUV - Universitat de València, Spain		
11:25-12:00	KN8	<u>Prof. Michael Fröba</u> , University of Hamburg, Germany "Templated synthesis of nanoporous materials in different morphologies"
12:00-12:20	OP19	<u>Dr. Gregorio Bottaro</u> , ICMATE CNR – Padova "Eu ³⁺ luminescence as a tool for the study of polar order evolution in Eu:BaZr _x Ti _{1-x} O ₃ ceramics"
12:20-12:40	OP20	<u>Mr. Charles Footer</u> , University College London, UK "Method to the magic; materials discovery of magnetic and dielectric nanoparticles for medical application"
12:40-12:50	FP5	<u>Dr. Alessandra Scano</u> , Dept. of Chemical Geological Sciences - University of Cagliari "Ultrasonication of Zn(II) salts and 4,4'-Bipyridine for the Synthesis of 1D-Coordination Polymers"
12:50-14:00	<u>Lunch Break (independent)</u>	

Afternoon Session

Chairman: Dipl.-Ing. Bernd Wittek, UMICORE AG – Hanau, Germany

14:00-14:35	KN9	<u>Dr. Patricia Hernandez-Fernandez</u> , Danish Technological Institute, Denmark "Up-scaling the production of functional nanomaterials with tailored properties using continuous supercritical flow synthesis"
14:35-14:55	OP21	<u>Dr. Helena Kaper</u> , Ceramic Synthesis and Functionalization Laboratory, CNRS/Saint-Gobain CREE, France "Electric arc fusion synthesis of perovskites and related materials"
14:55-15:15	OP22	<u>Dr. Francesca Deganello</u> , ISMN CNR – Palermo "Biperovskite nanocomposites prepared by solution combustion synthesis: a new concept for IT-SOFCs innovative materials"
15:15-15:25	FP6	<u>Ms. Silvia Mostoni</u> , Milano Bicocca University "Towards the up-scaled production of highly dispersed ZnO nanoparticles on silica as novel catalyst for the industrial rubber vulcanization process"
15:25-15:50	Coffee break (Aula A, via Marzolo, entrance)	
Chairman: Prof. M. Lourdes Calzada, Dept. of Materials for Information Technologies - ICMM-CSIC - Madrid - Spain		
15:50-16:10	OP23	<u>Dr. Enrico Ravera</u> , Dept. of Chemistry - University of Firenze "High resolution NMR of inorganic-protein composites"
16:10-16:30	OP24	<u>Mr. Danny Zanardo</u> , Dept. of Molecular Sciences and Nanosystems - Ca' Foscari University of Venezia "Synthesis of CuO/TiO ₂ photocatalytic nanocomposites by a modified precipitation approach"
16:30-16:40	FP7	<u>Dr. Thomas Ashton</u> , University College London, UK "Continuous hydrothermal synthesis of functional nanoceramic inks for printing applications"
16:40-16:50	FP8	<u>Mr. Stefano Marchesi</u> , Dept. of Science and Technological Innovation - University of Eastern Piemonte "On the physico-chemical properties of a novel class of saponite clays containing lanthanide ions in framework position"
16:50-17:00	FP9	<u>Ms. Martina Lippi</u> , Dept. of Chemistry, Materials and Chemical Engineering "Giulio Natta" - Milano Polytechnical "Highly dynamic and tunable behavior of 1D coordination polymers based on the bispidine ligand"
17:00-17:10	FP10	<u>Ms. Alexandra R. Groves</u> , University College London, UK "Continuous hydrothermal synthesis of perovskite titanates for use as oxygen reduction catalysts"
17:10-17:40	Poster Awards ceremony Closing Session (Aula A, via Marzolo)	

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Keynote Lectures

Low-temperature crystallization of solution derived metal oxide thin films assisted by chemical processes

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Keynote Lecture KN1

Significant efforts are devoted nowadays to the development of low-cost, large-scale solution methods for the low-temperature processing of metal oxide thin films on plastic substrates. Only some few years ago, amorphous oxide semiconductors have been successfully grown on plastics by low-temperature solution deposition methods.[1] More challenging is the preparation of crystalline oxide films with functional properties linked to their crystal structure, at temperatures compatible with their integration in flexible plastic substrates (≤ 350 °C). These oxides usually crystallize at temperatures over 600 °C, which has historically excluded them from their use in flexible electronics. This presentation shows an overview to the different solution strategies that our group has developed for the low-temperature fabrication of crystalline metal oxide films.[2] Most of these approaches are based in the use of UV light as an alternative energy source to induce crystallization by photochemistry. The efficiency of these UV-assisted solution methods for the low-temperature crystallization of metal oxide films on plastics is demonstrated for materials like the multiferroic BiFeO₃, the ferroelectric Pb(Zr,Ti)O₃ or the photocatalytic β -Bi₂O₃

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Ionic liquids for the low-T synthesis of inorganic nanocrystalline materials

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Keynote Lecture KN2

The synthesis of nanoscopic inorganic materials in ionic liquids (ILs) represents one of the various interesting properties and applications of ILs. In particular, ILs enable unusually low temperatures – compared to classical syntheses - being required for the nucleation of crystalline solids. Aside from the reduction of crystallization temperatures and grain sizes, ILs can even direct the crystallization to unusual and metastable structures such as the Bronze-type TiO₂(B) [1]. Meanwhile, the materials/substances being synthesized in ILs span a wide variety of unusual reactions/reactivity (e.g. of elemental phosphorus [2]) and complex inorganic compounds, including alloys and ternary oxides such transparent conducting oxides such as indium-tin-oxide (ITO) which are difficult to synthesize with high crystallinity by other methods [3]. The talk is intended to give an overview on reports about the synthesis of unusual compounds and nanoparticles in ILs, giving special focus on metal oxides and on the special role of the IL in directing the synthesis.

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Computational design of transition metal nanocluster catalysts for (electro)chemical reactions involving hydrogen

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Keynote Lecture KN3

The H2020-project CritCat (www.critcat.eu) aims to provide solutions for the substitution of critical metals, especially rare platinum group metals (PGMs), used in heterogeneous and electrochemical catalysis. CritCat explores the properties of ultra-small transition metal (TM) nanoparticles to achieve optimal catalytic performance with earth-abundant materials. The emphasis is on industrially-relevant chemical reactions and emerging energy conversion technologies in which PGMs play an instrumental role, particularly in the context of hydrogen energy.

CritCat aims to tailor optimal nanoparticle catalysts for selected (electro)chemical reactions based on atomistic simulations. The project includes large-scale DFT simulations of the relevant catalysts, substrates and model reactions (e.g. HER, acetylene semihydrogenation) using the latest computational methods. The DFT data is collected in full in a descriptor database and used for materials screening at later stages. We have also developed new algorithms based on machine learning for neural network (NN) force fields for generating catalyst structures, descriptor-based efficient hydrogen adsorption site scanning and prediction, and effective charge and electron energy level prediction based on coordinate files (xyz-format etc.). The new tools pave way for much more efficient catalyst simulations as they can produce catalyst structures and scan their reaction descriptors much more efficiently than DFT but with a similar accuracy. This will enable us to map promising materials in a virtual laboratory and circumvent the traditional trial-and-error approach.

Sustainable synthesis methods of smart nanocatalysts?

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Keynote Lecture KN4

Heterogeneous catalysis has grown from an art to a science. Numerous catalytic materials are being proposed every day in the literature, with surprising and exciting new reactivities being disclosed, and interesting novel concepts being proposed. For example, use of nanocrystals in CO oxidation turned out to be crucially dependent on the interfacial contact of the support (ceria) with the metal nanoparticle active sites [1], while valorization of biomasses were employed as reactants for catalysis by carbon-supported, Pt and PtCo nanocrystals (NCs) with controlled size and composition [2]. A particular type of structure is represented by nanosized core-shell phases, which proved to be superior catalysts in several catalytic reactions, such as methane combustion [3] as well as photocatalytic hydrogen evolution from biomass-derived substrates [4-6] or electrocatalytic water electrolysis [7] when integrated with multi-walled carbon nanotubes. Metal free nanocatalysts [8] and “intelligent” catalysts [9] are todays challenging but every day, nanotechnology applied to heterogeneous catalysts is creating new opportunities for important breakthroughs. The talk try to critically discuss the sustainability of some catalyst synthetic preparation procedure offering some perspectives.

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Miniemulsions as nanoreactors for the synthesis of inorganic nanomaterials for bio-applications and catalysis

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Keynote Lecture KN5

Polymeric nanocapsules offer the versatility to cover a wide range of mesoscopic properties for sophisticated applications. By means of the miniemulsion process, we can design custom-made nanocapsule systems for different purposes. The encapsulation and release of a great variety of payloads, ranging from hydrophobic to hydrophilic substances, have been successfully achieved in a highly controlled manner and with an unmatched high encapsulation efficiency.

Synthesizing nanocarriers with stealth properties, delivering 'payloads' to a particular tissue, and monitoring the effect of therapy remains a big challenge but is the prime prerequisite for any *in vivo* application. Critical issues here are the efficient encapsulation and protection of therapeutic agents, colloidal stability of nanocarriers against aggregation in blood induced by the adsorption of blood proteins and the composition of protein corona to achieve a long circulation time, and bioimaging. In this study, core-shell silica nanocapsules are synthesized as a platform with diverse possibilities of functionalizations. For instance, different organic liquids are used as core for the capsule. Fluorescent dyes can be labeled by either encapsulation in the core or covalently bonded in silica shell. Magnetic resonance imaging of silica nanocapsules can be achieved through embedding magnetic Fe₃O₄ nanoparticles. Colloidal stabilization of nanocapsules in blood circulation is achieved by using ethylene glycol-containing surfactants. The presented silica nanocapsule platform opens new opportunities for the development of multifunctional theranostic nanocarriers for biomedical applications.

In addition, when pressure is added to the system, the droplets act as tiny "pressure reactors" in which hydrothermal synthesis takes place. In this way, the advantages of the miniemulsion technique are combined with the possibilities of hydro- or solvothermal systems. The investigation of such novel synergy was the goal of synthesizing nanocarriers for catalysis and will be shown in detail in the presentation.

Watching solids crystallise and react using *in situ* analytical methods

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Keynote Lecture KN6

The discovery of new functional materials for various applications in energy and environmental fields requires exploration of a wide range of chemical reaction conditions and also an understanding of crystallisation pathways to allow some prediction in synthesis. We have been exploring solvothermal chemistry for the preparation of a wide variety of materials, from porous framework solids to ceramic oxides. We use *in situ* X-ray synchrotron methods at Diamond Light Source to follow crystallisation and understand materials' reactivity. I will describe some recent examples of our work, including [1] new metal organic frameworks, including some rare-earth materials whose crystallisation we have followed in laboratory-scale reactors using high energy X-rays to allow fine detail of the kinetics and structural evolution, [2]) the solvothermal formation of nanocrystalline spinel photocatalysts based on gallium oxide where *in situ* XRD shows the unexpected formation of transient layered hydroxides, and [3] the crystallisation of iridium oxide pyrochlores that have use as acid-resilient electrocatalysts for water splitting and where *in situ* XAFS allows us to examine the mechanism of catalysis by following changes in metal oxidation state under realistic conditions on applied potential in a electrochemical cell.

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- [3] “Time-Resolved Powder X-ray Diffraction of the Solvothermal Crystallisation of Cobalt Gallate Spinel Photocatalyst Reveals Transient Layered Double Hydroxides” D.S. Cook, Y. Wu, K. Lienau, R. Moré, R.J. Kashtiban, O.V. Magdysyuk, G.R. Patzke and **R.I. Walton**, *Chem. Mater.* **29** (2017) 5053–5057

Shape and 'impurities' of nanomaterials as a tool to control functional properties

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Keynote Lecture KN7

The dependency of materials properties on crystal size belongs to text-book knowledge, with semiconductor quantum dots or plasmonic nanoparticles as examples. Whereas for bulk semiconductors (e.g. silicon) it is clear, that full functionality can be accessed only after doping, most reports in the literature on nanomaterials deal with supposedly pure compounds. The role of intentional (doping) or unintentional (impurities) introduction of heteroelements into semiconductor nanostructures will be debated.

A further argument for features differing at the nanoscale is the increased surface to volume ratio. Because the surfaces correlate in some way to the lattice planes (hkl) of the crystal (Fig. 1), meanwhile, one has realized, the abundance and type of these surfaces has a major influence as well. The abundance and type of surfaces is determined by the shape of a nanocrystal, which is why shape-property correlations exist.^[1] The morphogenesis of nanoparticles will be discussed first, followed by the analysis of representative examples for shape-property correlations. One feature influenced heavily by shape is their ability for self-assembly and superstructure formation.^[2-3] Collective phenomena may then emerge from these superstructure, which is a topic related to the field of particle-based materials.

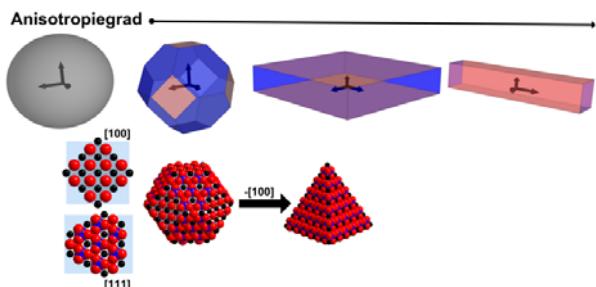


Fig. 1. Particle shape-surface correlations.

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Templated synthesis of nanoporous materials in different morphologies

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Keynote Lecture KN8

Nanoporous materials play an important role in the field of heterogeneous catalysis, separation, sorption, drug release, energy storage and many more. Very often a well-defined porosity with uniform pore sizes, high surface areas and certain pore topologies has to be combined with a special morphology like spherical (nano)particles, monoliths, thin films or just powders. In general, the synthetic approach to achieve such properties is the usage of templates which can be small molecules, supramolecular aggregates (e.g. lyotropic liquid crystals or polymers), hard spheres or even solvent mixtures which pass through a phase separation. In all cases the structure-directing effect is determined by the strength of the interactions between the template and the inorganic or organic/inorganic hybrid component. These interactions which can be of strong ionic or covalent nature or just van-der-Waals forces or H-bridges can be adjusted for the respective desired type of nanoporous material. With respect to the way the template introduces porosity one distinguishes between endo-/exo- and hard-/soft-templates.

In this contribution we will present various ways to synthesize nanoporous silica, carbon and organosilica materials with spherical morphologies (nanoparticles, hollow spheres and yolk/shell particles), monoliths and inverse opal structures. In addition a short introduction into the concepts of pseudomorphic transformation and ionotropic gelation will be given [1-4].

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Up-scaling the production of functional nanomaterials with tailored properties using continuous supercritical flow synthesis

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Keynote Lecture KN9

We present here an up-scalable flow synthesis method capable of producing nanomaterials with very precise control of crystallinity, particle size, stoichiometry and spatial distribution onto high surface area substrates. Supercritical fluids are interesting because they share properties from gaseous as well as liquid phases. They offer the opportunity to manipulate different properties of the reaction media as density, viscosity or diffusivity by controlling the pressure and temperature. Our continuous solvothermal flow reactors allow us to bring solvents into the supercritical phase, resulting in rapid mixing and heating of the reactants that will cause instantaneous nucleation of nanoparticles. The use of supercritical fluids in a flow enables very precise control of the nanomaterial properties, allow synthesis of particles directly onto support nanomaterials, and our reactors can produce up to 500 g/h of nanomaterials [1].

We have demonstrated the production of carbon supported metallic nanoparticles for PEM fuel cell applications with high activity and stability. This includes pure Pt, but also alloys such as Pt_xNi and Pt_xCo catalysts with oxygen reduction activities reaching 1.5 A/mg_{Pt} at 0.9V, surpassing by far the DOE target for 2020 of 0.44 A/mg_{Pt} [2]. Various oxides have also been prepared, such as γ -alumina with very high surface areas of ca. 500 m²/g, produced in a single step. γ -alumina is used for many industrial applications, e.g. as support in e.g. diesel oxidation catalysts. For this application, we have incorporated various metals, e.g. Pt, Pd and Fe, resulting in very active catalysts with significant PGM saving potential. Our method has also been used for the preparation of mixed oxides, such as ceria-zirconia doped with lanthanides, with high surface area, oxygen storage capacity and stability. used as washcoat in three-way catalysts for e.g. gasoline-powered vehicles.

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Oral Presentations

A "three-in-one" approach to induce the low-temperature crystallization of BiFeO₃ thin films

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Oral Presentation OP1

Functional thin films based on complex metal oxides show crystallization temperatures usually over 600 °C. This has historically excluded them from a direct integration into flexible electronic systems, since their processing temperatures are several hundred degrees above the values that polymeric substrates can withstand (≤ 350 °C). The versatility of wet chemical methods has recently allowed the exploration of unconventional crystallization pathways for metal oxides thin films and makes them fundamental in the search of low-temperature methods [1]. In this work, the combination of three different but complementary low-temperature strategies has made possible the crystallization of photoferroic BiFeO₃ thin films at temperatures below 350 °C. First, the synthesis of photoactive species by wet chemistry opens the door for a wide range of photochemical reactions to be induced in the system by UV light (photolysis, ozonolysis, condensation, densification and even crystallization). Second, the optimization of the chemical system by metal precursors with additional roles as oxidizing and fuel agents may provide an internal energy supply by combustion reaction responsible for obtaining the respective product (the metal oxide) at lower temperatures. Third, the design of molecular precursors with a structure that closely resembles the crystalline structure of the corresponding metal oxides makes this conversion to proceed with a low energy input. As a consequence, crystalline BiFeO₃ thin films were grown on flexible plastic showing an adequate ferroelectric and photovoltaic response. With flexibility, a new dimension for functionality is therefore added to this important family of advanced inorganic materials.

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A sol-gel approach for the production of exhaust catalysts

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Oral Presentation OP2

Catalytic converters for the abatement of pollutants in engine exhaust gases (“exhaust catalysts”) are traditionally manufactured in a simple fashion: A precursor compound of a precious metal is mixed with a thermally stable oxide. With this suspension (“the washcoat”) a monolithic ceramic carrier is coated. The requirements for the oxides used in this process are to be thermally stable with a sufficiently high internal surface area in order to increase the amount of catalytically active sites within the catalyst. The most commonly used metal oxide for exhaust catalysts is alumina. In order to produce $\gamma\text{-Al}_2\text{O}_3$ possessing the required high surface area, $\gamma\text{-AlO(OH)}$ (Boehmite) is being heat treated. During the coating process the washcoat is dried and again heat treated.

This presentation discusses the use of aluminum-containing colloidal solutions being used as a starting point for the production of a washcoat avoiding partially the intermediate energy-intensive heat treatment deemed necessary to produce high surface areas.

Electrochemical and photochemical deposition of MnO_x on porous ZnO scaffolds

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Oral Presentation OP3

ZnO is being discussed as a possible photocatalyst. However, the applicability of ZnO as catalyst is strongly limited to high energy radiation due to its large bandgap (3.3 eV). By coupling ZnO with 3d metal oxide clusters (e.g. MnO_x) light absorption can be enhanced. MnO_x is a good thermocatalytic material [1] and environmentally friendly [2].

The starting point of our investigations towards MnO_x/ZnO composite materials is two different semiconductor model systems. The first model system is a ZnO nanowire array grown by electrodeposition in a solution containing ZnCl₂ and KCl. The nanowire diameter and length can be tuned either by the concentration of KCl or by the deposition time. The ZnO nanowires have dimensions of 500 nm – 2 µm in height and of 25 nm – 300 nm in diameter [3], [4]. We compare this array of oriented nanowires to a random particle network built up by ZnO nanocrystals (14 nm) prepared by chemical vapour synthesis [5].

The morphological particularities of the two ZnO films give rise to different electrical properties. Whereas the electron transport in ZnO nanowires is directional and follows the axis of the nanowire, it follows a random path in ZnO nanoparticle networks. In addition, band bending within single ZnO nanowires occurs due to the macroscopic dimensions of the nanowires, whereas internal electric fields are absent in nanoscopic ZnO nanoparticles.

We used electro- and photodeposition for growing MnO_x clusters and thin shells on ZnO nanowire arrays and on nanoparticle films out of a KMnO₄ solution. The impact of deposition parameters (potential, time) on the distribution of MnO_x clusters on the ZnO surface is evaluated in the light of the different electronic and morphological properties of the two model systems. Furthermore, we investigate the impact of thermal annealing on the structural, morphological and electrochemical properties of the films.

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Continuous hydrothermal flow synthesis of lithium-nickel rich NMC layered materials for lithium-ion batteries

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Oral Presentation OP4

In the last few decades the growing pressure on resources and the environmental crisis have dramatically increased. This has led to a major research to develop energy-storage technologies, especially those based on lithium-ion batteries (LIBs) which are expected to be used in device applications, such as stationary energy storage, smart grid, electric transportation, etc. LiCoO₂ (LCO) has been the first and most commonly employed cathode in portable electronics. However, the LCO cathode was found to be unstable in a highly delithiated state with high voltages of above 4.3 V and have a relatively small amount of charge, up to 160 mAhg⁻¹.

These issues have been recently overcome by introducing Ni and Mn to the structure of LCO layered materials, Li_{1+x}(Ni_{1-y-z}Mn_yCo_z)_{1-x}O₂. Replacing Co with Ni in this layered structure results in higher utilisation of lithium, increasing its theoretical capacity to 275 mAhg⁻¹, with almost 80% reversible extraction of Li in the host structure. In the last few years a range of different Ni-based derivatives has been studied, being found that these cathode materials could achieve energy densities of 800 WhKg⁻¹.

In this work, rich Ni-based derivatives, namely NMC811 (80 % Ni) and NMC622 (60 % Ni) have been synthesised using a two-step method approach. Firstly, Ni_{1-x-y}Mn_xCo_yO nanoparticles were synthesised by continuous hydrothermal flow synthesis methods (CHFs), a scalable and sustainable route towards the rapid synthesis of nanomaterials. Subsequently, these nanoparticles were lithiated at 850 °C for 5 h. The use of this synthetic approach resulted in the formation of NMC cathode materials with reduce particle size, ranging from 1 to 2 µm, which would allow virtually full charge capacity. These rich Ni-based NMC derivatives have showed capacities of 170 mAhg⁻¹ and 150 mAhg⁻¹ (4.6 V) for NMC811 and NMC622, respectively, with remaining capacities of 150 mAhg⁻¹ and 137 mAhg⁻¹ at a specific current of 0.75 Ag⁻¹. Because of their performance at high rate, good stability and small particle size, the rich Ni-based NMC derivative materials presented in this work are of interest for Li-ion batteries applications.

The importance of Cu(I) intermediates in self-reducing molecular inks for Cu deposition

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Oral Presentation OP5

Printed Cu features are applied in several electronics e.g. RFID antennas, sensors. For plastic substrates in flexible applications, the thermal budget is strictly limited <150°C. Recently, amine-formato-copper(II) coordination compounds are applied in molecular self-reducing inks, which advantageously decompose below 150°C [1,2], much lower than pristine copper formate (225°C). Hypotheses to explain this temperature decrease have been proposed, but were never worked out in detail.

Here, we focus full attention on understanding the decomposition of amine-formato-copper(II) complexes, for a selection of amines. First, these complexes' structure was determined by single-crystal XRD, EXAFS, FTIR and Raman spectroscopy. The reduction mechanism during heating was studied by in-situ XRD and in-situ XANES. The latter spectra were analyzed by principal component analysis, revealing Cu(I) complexes formed as intermediates and their structure. By comparison of the structures of the starting Cu(II) complex and intermediate Cu(I) compound, a correlation was found between similarity in their structure and decomposition temperature. Based on these experiments, we believe the Cu(I) intermediate is the most important factor in rationalizing the lowering of the decomposition temperature for self-reducing amine-formato-Cu(II) complexes. This in-depth understanding, lays foundations for basic design rules of efficient inks, thereby enhancing the prospects for applied research of printed electronics.

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Precise and scalable production of nano-catalysts by nanocluster beam deposition

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Oral presentation OP6

Heterogeneous catalysis is a vital and growing area thanks to its traditional applications and diverse possibilities in clean energy technology, environmental pollution reduction and so on. One of the main challenges is the control of both composition, structure, size and morphology of the catalyst particles involved in the reactions. The best current catalyst particles rely on critical materials, such as the platinum group metals, that need to be reduced or replaced because of their scarcity and cost and to avoid supply issues.

Pt-X bimetallic clusters have been produced via a gas-phase, ligand free synthesis route before deposition onto catalyst supports, with a broad range of composition and atomic structures in order to investigate the effect of these parameters on the catalytic performance. The findings of these studies can be exploited with a new technology for clusters production developed by the Swansea group, the Matrix Assembly Cluster Source (MACS), with the possibility to scale-up the cluster production rate to the gram scale [1].

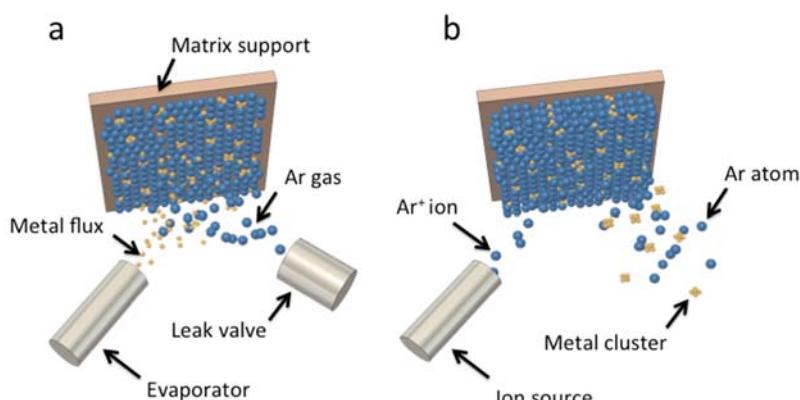


Figure: Schematic diagram of reflection mode in MACS. The matrix is formed by vaporizing cluster material atoms and rare gas atoms (e.g. Ar) condensed onto the matrix condensation plate ($T < 20K$) at the same time (a). Clusters are produced by high energy Ar ions sputtering the matrix (b).

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Unconventional synthesis of titanium-tetrapyrrole films at TiO₂(110): a computational and experimental approach

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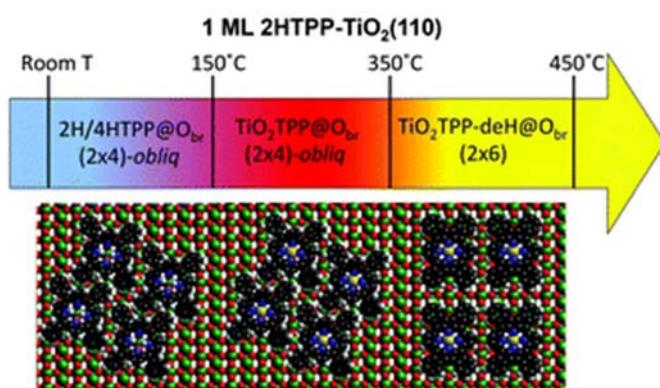
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Oral Presentation OP7

Surface modification with functional films is a popular way to improve the properties of inorganic particles for a number of applications. A well-known case is that of dye-sensitized cells, where absorption of the solar spectrum in the visible and near-infrared region of metal oxides such as TiO₂ or ZnO is enhanced by films of metal complexes with suitable HOMO-LUMO gaps. It is generally assumed that in these heterostructures the supporting metal oxide is chemically innocent, and that molecules are adsorbed – chemically or physically – unchanged. In contrast to this picture, we show that, starting from room temperature, TiO₂ actively interacts with adsorbed porphyrins, exchanging atoms, and giving rise to self-hydrogenations, self-metalations, and dehydrogenation reactions, which ultimately bring to the synthesis of films of exceptionally high thermal stability (up to 450 degrees C), potentially useful for sensors

and photocatalysis applications in harsh environments. Furthermore, our findings indicate that metal exchange with the very reactive Ti atoms must be taken into account when designing porphyrin-sensitized solar cells, because the critical temperature for the onset of self-metalation is very close to the normal operating temperature of photovoltaic devices.



"Pigments of life", well-suited molecules to look into the metal \square ligand symmetry □

Restricted covalency

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Oral Presentation OP8

X-ray absorption spectroscopy (XAS) of transition metal (TM) complexes is recognized as a tool able to probe, site-selectively, the empty frontier MOs, the TM coordinative environment, the ligand-field splitting, the oxidation states and, in general the nature and the strength of the TM–ligand bonding in TM complexes. L_{2,3}-edges XA spectra contain a huge chemical information, but a detailed theoretical analysis is needed to extract it. The L_{2,3}-edges XA simulated spectra presented have been obtained by using the Restricted Open shell Configuration Interaction with Singles method, which includes spin orbit coupling and relativistic effects. Numerical experiments have been carried out to investigate the TML_{2,3}-edges spectra of a huge number of systems, which spread from single molecules (TM(acac)₂ (TM = Mn, Co) [1,2], TM(acac)₃ (TM = Cr, Mn, Fe) [2,3]) to 2D complex systems (VPc and VXPc (X = O, I) [4,5], FePc/FePc(η_2 -O₂) [6] and CuPc/CuTPP [5,6,7]).

The goals of these systematic studies were i) to revealing the role played by the central TM ions and by its oxidation state and its environment in determining the spectral features, ii) to provides an understanding of the electron transfer pathway ruling the catalytic oxygen reduction reaction of FePc on Ag(110) and iii) to quantify the amount of different species that contribute to the same XA spectrum. Relevant trends for L₃-edge XA spectra are the lower energy side is characterized by TM \rightarrow TM transitions, while the higher energy one involves metal to ligand charge transfer transitions.

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**Preparation of advanced nanostructured electrodes
for energy and chemistry transition**

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Oral Presentation OP9

Driven from competitiveness in a changing economic world with an increasing transition to renewable energy, chemical and refinery production are in a major transition phase to go beyond fossil fuels (as main raw materials and energy source) and to increase sustainability, besides to increase energy efficiency and reduce waste.^[1] One of key areas related to these aspects is generated by the need to develop advanced nanostructured electrodes for photo- and electro-catalytic applications,^[2] and particularly for photo-electro-catalytic (PEC) devices. In this respect, design of the PEC cells in terms of applicability and aspects such as low-energy-intensive products recovery, imposes a series of constraints in terms of electrode characteristics which are typically not considered.^[3]

This lecture will discuss some aspects of the preparation, characteristics, performances and engineering of photo- (anode) and electro-catalytic (cathode) electrodes for PEC fuel cells, for both water splitting and CO₂ reduction. TiO₂-based anode electrodes and nanocarbon-based and hybrid cathode electrodes, the latter for the reduction of CO₂, will be discussed, after briefly commenting the challenges for nanostructured catalytic electrodes deriving from the on-going chemistry/energy transition and some of the requirements deriving in terms of electrode design.

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New route for the production of furan 2,5-dicarboxylic acid with a CeO₂ supported Au catalyst

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Oral Presentation OP10

Large-scale production of commodity chemicals from renewable feedstock has received significant attention as a means of diminishing our current dependence on fossil fuel resources and developing a sustainable chemical industry. Furan 2,5-dicarboxylic acid (FDCA), identified as one of the top 10 bio-based chemicals by the U.S. Department of Energy, has been widely recognized as a suitable replacement for petroleum-derived terephthalic acid for polymer applications and can be synthesized by aerobic oxidation of 5-(hydroxymethyl)furfural (HMF) using a supported metal catalyst. FDCA or its methyl ester with bio-based ethylene glycol can be polymerized into poly(ethylene 2,5-furandicarboxylate) that is superior to poly(ethylene terephthalate) in terms of its low permeability for various gases, excellent processing properties, and high tensile strength. However, the large-scale FDCA production of HMF has been largely limited by the formation of solid humin as a by-product, which prevents continuous operation of feasible batch and flow-type processes. Here we report that aerobic oxidation of HMF-acetal with 1,3-propanediol enables selective FDCA formation (90-95%) from highly concentrated solutions (10-20 wt%) using a CeO₂-supported Au catalyst. The reaction of HMF with 1,3-propanediol produces an HMF-acetal derivative that exhibits excellent stability toward thermal decomposition and self-polymerization of HMF in concentrated solutions. Kinetic studies supported by density functional theory calculations identify two crucial steps in the reaction mechanism, i.e., the partial hydrolysis of the acetal into 5-formyl-2-furan carboxylic acid involving OH⁻ and Lewis acid sites on CeO₂, and subsequent oxidative dehydrogenation of the in situ generated hemiacetal involving Au nanoparticles. The present results represent a significant advance over the current state of the art, overcoming an inherent limitation of the oxidation of HMF to an important monomer for biopolymer production.

Solvent-free mechanical synthesis of Pd/CeO₂ catalysts for methane abatement

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Oral Presentation OP11

The general concern for global pollution is pushing towards novel and solvent-free synthesis approaches, which are regarded as valid alternatives to wet procedures [1]. Here we describe the preparation of a novel Pd-ceria formulation (1 wt% Pd) by simple, low intensity milling of Pd and CeO₂ powders. Briefly, Pd black (Aldrich) and CeO₂ powder were milled together in a ball mill at 15 Hz for 10 minutes and using one zirconia ball [2]. The procedure results in a unique Pd-ceria arrangement in which an amorphous shell, comprised by Pd and Ce atoms, surrounds ceria nanoparticles (Fig. 1a). The amorphous shell is generated by the dissolution of Pd clusters into the ceria lattice (Fig. 1b).

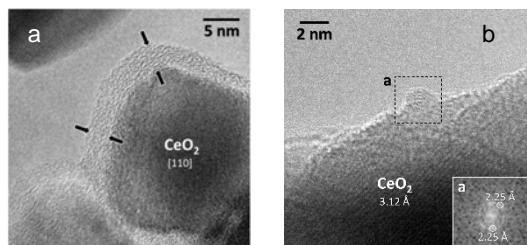


Figure 1. HRTEM images of milled Pd/CeO₂ catalyst

The catalyst so obtained was tested for lean methane oxidation, revealing to be much more active than conventional Pd/CeO₂ made by incipient wetness impregnation. The reaction rate measured for the milled sample at 623 K was of 212 μmol CH₄/g_{Pd}*s vs 32 μmol CH₄/g_{Pd}*s for the impregnated catalyst. The outstanding performance of the milled sample has been ascribed to the strong contact at nanoscale between Pd and ceria generated by the milling procedure.

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Colloidal synthetic strategies for the microencapsulation of inorganic phase change materials

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Oral Presentation OP12

Phase change materials (PCMs) are materials with the ability to store thermal energy in form of latent heat during a phase change, often a solid–liquid transition. Hydrated inorganic salts can act as efficient PCMs with a high storage capacity in a wide range of temperatures, but their application suffers of limitations due to problems of phase segregation, supercooling or corrosion of the surrounding media. In this context, micro- and nanoencapsulation is a useful approach [1].

In this work, we present synthetic strategies based on interfacial miniemulsion polymerization for encapsulating inorganic PCMs. We synthesized and post-functionalized magnetite and cerium(IV) oxide nanoparticles that play the role of a surfactant during the capsule formation, according to a so-called Pickering stabilization. The final capsules are hybrid in nature, with a polymer component and incorporated metal oxide nanoparticles, with structural and functional character.

The ability to store thermal energy of the different systems prepared was studied by differential scanning calorimetry (DSC). Supercooling problems (i.e., crystallization at significantly lower temperature than the melting point), common in hydrated salts, were corrected by the co-encapsulation during the synthesis of small amounts of a nucleating agent. The storage of thermal energy is efficient and reproducible after a large number of cycles.

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Characterisation of plasmonic copper sulphide nanocrystals containing solid lipid nanoparticles and determination of their concentration

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Oral Presentation OP13

Inorganic nanocrystals (NCs) based nanovectors offer the potential for new and innovative drug delivery systems for a targeted transport of drugs towards tissues affected by most aggressive disease including cancer. Diagnostic and therapeutic applications require, for both *in-vitro* and *in-vivo* investigation, the determination of the maximum cellular dose of these nanovectors [1] that is also mandatory for any regulatory approval [2]. Accurate determination of the nanovector concentration is not a trivial issue and currently there is a lack of experimental methods recognized as general and reliable [3]. In this work, we propose an approach for the determination of the concentration of a solid lipid nanoparticle (SLN) nanovector encapsulating photoactive copper sulphide ($Cu_{2-x}S$) NCs characterized by a tunable localized surface plasmon resonance (LSPR) in the biological transparent near-infrared (NIR) spectral region for photothermal therapy. Here, $Cu_{2-x}S$ NCs with a narrow size distribution and an intense LSPR in the second biological window have been synthesized by hot injection method and they have been encapsulated into SLN prepared by a hot homogenization technique using a mixture of lipids, triglycerides and phospholipids. A calculation method based on Mie-Drude theory using as input data resulting from spectroscopic and dimensional investigation for the $Cu_{2-x}S$ NCs and NCs containing SLNs has been successfully implemented and applied for the determination of the nanovector concentration. The results are in agreement with experimental data and the proposed approach hold a great potential for determining the concentration of plasmonic NCs based nanovectors.

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Characterization of N-doped hydroxyapatite nanocrystals through SAXS and synchrotron WAXS Total Scattering Methods

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Oral Presentation OP14

Hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, or HA), the mineral constituent of bones and teeth, is one of the most studied biomimetic materials for its biocompatibility and versatility. In fact, the ability of incorporating a number of exogenous ions into its crystal structure makes HA an interesting material to achieve desired material properties through designed synthetic pathways. This is particularly effective if HA is confined at the nanoscale. In this study, HA-based nanocomposites [1] (a mixture of amorphous – ACP – and nanocrystalline components) where synthesized according to green chemistry principles and doped with N-rich compounds, aiming at developing innovative, more efficient and sustainable fertilizers for agriculture application. Nanocomposite characterization was carried out through both conventional physico-chemical analyses and advanced scattering techniques, such as synchrotron-based Wide Angle X-ray Total Scattering (WAXTS), coupled to advanced modelling based on the Debye scattering equation [2], Small Angle X-ray Scattering (SAXS) and Static and Dynamic Light Scattering (SLS/DLS). The in-depth characterization provides information on the structure-properties relation, enabling a controlled macronutrient release by modulating the size, structure and composition of nanoparticles through a synthesis-by-design approach, making them a promising smart and sustainable fertilizer.

This work was partially supported by Fondazione Cariplo (HYPATIA, No. 2016-0648).

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[2] Cervellino et al. 2015 (DOI: 10.1107/S1600576715020488)

In-situ/operando investigation of heterogeneous catalysts with XAS

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Oral Presentation OP15

Being element-specific, XAS spectroscopy allows the selective investigation of the active metal sites in heterogeneous catalysts with no or negligible interference from the environment (support and/or reaction mixture). Accordingly it can be exploited under actual reaction conditions and can be successfully applied to heterogeneous and homogeneous systems and to concentrated samples and highly diluted/non homogeneous systems. Differently from XRD and NMR, XAS also allows the investigation in solution of metal species with short-range order and fine nanoparticles. Finally, space (at micrometer scale) and time resolved (at subsecond scale) investigation is possible due to collimated beam and the availability of techniques, such as quick EXAFS, respectively. In this contribution, the potential of in-situ/operando XAS for the investigation of heterogeneous metal catalyst is shown for the direct synthesis (DS) of H₂O₂ and for Heck and Suzuki reactions, both in the liquid phase. In the DS a supported nanostructured Pd or a bimetallic Pd catalyst is used to promote the selective hydrogenation of O₂ to H₂O₂. The Pd K-edge in-situ investigation, using a home-designed and made plug flow catalytic cells, was carried out to identify intermediate species and disclose the role of Br⁻ ions as selectivity enhancers. The Heck and Suzuki reactions are also catalyzed by palladium catalysts and are of paramount importance in the synthesis of complex organic molecules. The nature of the active species, especially when a supported metal (pre)catalyst is used, was the subject of controversy in the first decade of 2000's. Time and space resolved XAS investigation provided important information in this context confirming the previous general view on the role of the leached Pd species in these reactions.

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Sustainable fabrication of high temperature SrTiO₃-based catalysts

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Oral Presentation OP16

Sustainability has become an all-round concept, which not only considers the exploitation of renewable energy sources to reduce the consumption of fossil fuels, but also involves the conception, production and processing of energy materials.

Ternary oxides are considered promising materials for the substitution of precious platinum-group-metal catalysts. These systems can be prepared by hydrothermal process, a green, low-temperature approach. However, owing to the mild synthesis conditions such nanostructures are unstable at the high temperatures typical of redox catalysis and need therefore to be stabilized via sintering. In the ceramic engineering, electric-field assisted sintering, or flash sintering, has recently emerged as novel, environmental-friendly technology able to massively reduce the process time and cost with respect to conventional treatments.

Herein, we present the effect of flash sintering on the microstructure and catalytic properties of SrTiO₃ and La_{0.1}Sr_{0.9}TiO₃ nanoparticles. We could show that the fast process kinetics along with high-voltage current flow has a strong impact on the materials' grain growth and defect composition. More importantly, catalysis experiments exhibited exceptionally high activity for flash sintered perovskites, presenting full conversion of methane at 800°C and twice as high than for conventionally sintered materials.

Luminescent nanomaterials prepared by microwave-assisted hydrothermal synthesis: two interesting cases

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Oral Presentation OP17

Microwave-assisted hydrothermal synthesis (MAHS) is a relatively recent route to prepare nanomaterials that can be interesting in many applications [1, 2]. The advantages of this technique are a homogeneous heating, short reaction times and ease of scaling up for industrial synthesis of functional nanomaterials.

Two types of nanomaterials prepared by our group using MAHS will be considered and discussed: carbon dots and lanthanide doped upconverting fluoride nanoparticles. Some results on the morphological properties vs the synthesis conditions will be analyzed. The luminescence properties of the carbon dots will be presented. Moreover, upconversion properties, Stokes emission in the visible and infrared regions and thermometric performances in the biological windows for lanthanide doped fluoride nanothermometers will be presented, indicating that these nanomaterials can be very useful in nanomedicine.

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Facile microwave hydrothermal synthesis of multiferroic micronised particles

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Oral Presentation OP18

Multiferroic materials, single phase bismuth ferrite perovskite-type structures, are acquiring interest in information storage, sensors applications and photocatalytic degradation as they exhibit ferromagnetic and ferroelectric properties in a certain temperature range [1-2]. The synthesis of these complex oxide systems still remain a challenge due to the multiplicity of oxidation states, morphologies and phases. Nowadays, most perovskite-based materials are prepared by solid-state reactions starting from the corresponding oxides at temperature above 1000 °C. Other preparation procedures include sol-gel method, Pechini method, auto combustion, chemical co-precipitation method including solvothermal and hydrothermal synthesis [3,4]. However, one of the major underlined problem is the preparation of bismuth ferrite perovskites as single phase: as reported in literature the main phase is often obtained in presence of secondary phases in both the micrometre-sized and nanostructure regions [3,4]. The microwave hydrothermal synthesis route is used as an alternative way to give compounds of high purity. In particular, in this work the microwave assisted hydrothermal method is applied to successfully synthesize bismuth ferrites (BiFeO_3 , also commonly referred to as BFO in materials science) and lanthanum doped (BLFO, $\text{Bi}_{1-x}\text{La}_x\text{FeO}_3$ where $x = 0, 0.15, 0.30$ and 0.45) in pure-phase. The growth mechanisms of these multiferroic crystallites are discussed in details. The influence of process parameters, such as precursor ratio, mineralizer concentration, temperature and time on phase formation, particle size distribution and morphology, are investigated in details. Finally, both BFO and BLFO powders morphology is characterized by ESEM and TEM. The existence of the single-phase perovskite structure for all the prepared compounds is evaluated by the X-ray powder diffraction patterns.

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Eu³⁺ luminescence as a tool for the study of polar order evolution in Eu:BaZr_xTi_{1-x}O₃ ceramics

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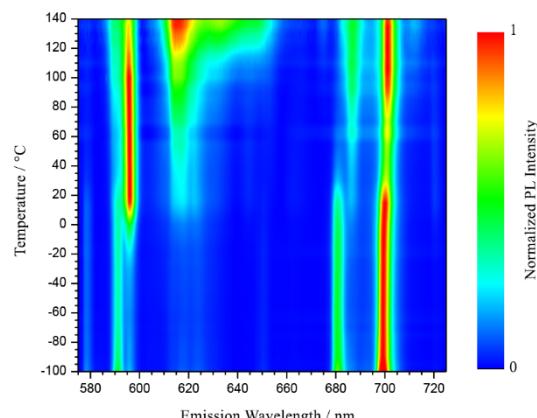
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Oral Presentation OP19

BaZr_xTi_{1-x}O₃ (BZT) solid solutions with perovskite structure show a series of phase transitions and a progressive evolution of ferroelectric order, from long-range typical of ferroelectrics ($x = 0\text{-}0.15$), to short-range order typical of relaxors ($x \geq 0.25$) via a diffuse transition behavior ($x = 0.15\text{-}0.25$). Paraelectric non polar state is instead observed in neat BaZrO₃. The trivalent europium ion (Eu³⁺) is well known for its bright red luminescence and for the capability to act as unique and powerful local structural probe. In this framework, we have investigated the photoluminescence (PL) of dense BZT ceramics doped with Eu³⁺ (Eu_yBa_{1-y}Zr_xTi_{1-x-y/4}O₃; $y = 0.01$, $x = 0, 0.05, 0.15, 0.30, 0.50, 0.70, 1$), in the -100 to 140°C temperature range. PL spectra underwent to significant shape and intensity variations as function of both composition and temperatures, which can be correlated with the nature (long-range or short-range) of polar order. The strong variation of the PL spectra induced by temperature change can be exploited to develop ratiometric self-calibrating luminescence thermometers working from room temperature down to liquid nitrogen.

Temperature dependence of Eu³⁺ emission in Eu³⁺ doped BaTiO₃



Method to the magic; materials discovery of magnetic and dielectric nanoparticles for medical application

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Oral Presentation Op20

Continuous flow hydrothermal synthesis (CHFS) is a scalable and sustainable route towards the rapid synthesis of nanomaterials, applicable to a diverse range of applications. Metal salts are intimately mixed with supercritical water ($T > 374\text{ }^{\circ}\text{C}$, $P > 22\text{ MPa}$) in a patented confined jet mixer, inducing instantaneous heating and mixing of the two fluids at the mixing point such that the solubility of the metal source decreases, and the nucleation of nanoparticles (oxides, titanates, ferrites, metals) ensues. Reaction times are $< 5\text{ s}$ and nucleation and growth processes can be controlled and manipulated by varying process parameters. This novel and exciting technique has been employed in this project as the foundation for a materials discovery methodology which has its foundations in pharmaceutical companies' drug discovery efforts and explores the capabilities of QinetiQ and UCL in order to discover interesting and novel candidates for use in electromagnetic applications such as that in remedial healthcare and treatment of illnesses such as cancer. This ambitious project involves the employment of a variety of different fields of science including: materials synthesis; process engineering; chemical characterisation; physical testing; mass data collection and storage; data mining; and macro analysis. This methodology and its associated work mean that a new level of understanding can be developed of the relationship between structure and electromagnetic response. The first 18 months of this PhD programme have been successful in synthesising and electromagnetically characterising over 700 nanoparticle candidates.

Electric arc fusion synthesis of perovskites and related materials

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Oral Presentation OP21

When going from lab scale synthesis to industrial production, one of the main questions is whether characteristic properties of the lab-synthesized materials can be retained during upscaling. In this work, two synthesis methods for the preparation of perovskites and related materials are compared: electric arc fusion (EAF) as an industrially relevant synthesis method and Pechini synthesis as a typical lab technique. The materials of choice are the perovskite $\text{CaTi}_{0.9}\text{Fe}_{0.1}\text{O}_{3-\delta}$ and the Brownmillerites $\text{CaFeO}_{2.5}$ and SrFeO_x . The materials will be evaluated for the oxygen ion conductive properties and catalyst support characteristics. Despite the low surface area of below $1 \text{ m}^2/\text{g}$ for $\text{CaTi}_{0.9}\text{Fe}_{0.1}\text{O}_{3-\delta}$ obtained from EAF, oxygen ion mobility is even higher than for the Pechini synthesized materials.[1] The situation is slightly different for the Brownmillerites. In the case of $\text{CaFeO}_{2.5}$, the lower surface area of the EAF-synthesized materials leads to oxygen mobility taking place at higher temperature and lower catalytic performance. For SrFeO_x , more reduced materials are obtained for the EAF synthesis, leading to higher oxygen mobility. These three examples show that in principal, lab scale synthesis can be transferred to industrial production such as EAF. However, not always the same characteristics are retained, and even novel properties can be found.

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***Biperovskite nanocomposites prepared by solution combustion synthesis: a new concept for
IT-SOFCs innovative materials***

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Oral Presentation OP22

Intermediate Temperature Solid Oxide Fuel Cells (IT-SOFCs) are envisaged as one of the most powerful devices for providing clean energy with high efficiency. Today, an important challenge for their development as eco-friendly technology is to obtain a cathode material with high oxygen reduction ability below 800°C. Perovskite-type compounds, like Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-δ} (BSCF), with cubic structure, and La_{1-x}Sr_xCo_{1-y}Fe_yO_{3-δ} (LSCF), with orthorhombic ($y \geq 0.5$) or rhombohedral ($y < 0.5$) structure, are among the most promising cathode compositions. Solution combustion synthesis (SCS) is an efficient methodology for the single-step synthesis of nanostructured and ultra-fine perovskite-type compounds with complex compositions and targeted microstructural properties. Herein, a Ba, La, Sr, Co and Fe-containing all-perovskite nanocomposite, here named “*biperovskite*”, was created by SCS dissolving the metal nitrates precursors in water with a sucrose-polyethylene glycol fuel mixture and characterized for application as IT-SOFCs cathode materials. After annealing at 900°C, Rietveld analysis applied to XRD patterns and HR-TEM disclosed a nanostructured powder composed by a BSCF-type (Pm-3m) and a LSCF-type (R-3c) structure. The sucrose-polyethylene glycol eco-friendly mixture granted that all the metals remained trapped in the correct positions forming a gel network characterized by a cage-like structure. As evidenced by TGA, H₂-TPR and XPS measurements, the high reducing power of sucrose-polyethylene glycol fuel mixture promoted an oxygen vacancy-rich configuration, which is essential for an optimal oxygen exchange with air and a suitable ionic transport. Electrochemical characterization performed by impedance spectroscopy, on a symmetrical membrane electrode assembly with a Ce_{0.8}Sm_{0.2}O_{2-x} electrolyte, revealed area specific resistance (ASR) values of 0.0177 Ω·cm² at 780°C and 0.0187 at 600°C, which are competitive with those of perovskite-type cathode materials reported in the literature.

High resolution NMR of inorganic-protein composites

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Oral presentation OP23

We have demonstrated that high quality SSNMR spectra can be obtained from immobilized proteins, and that this information can lead to the understanding of their structural features in these artificial but functional environments.^[1,2] Inorganic/protein composites have peculiar properties with respect to the usual samples for biomolecular or materials NMR, because the protein and the material affect each other. We have further demonstrated that ¹H detection^[3] and DNP^[4] can mitigate the sensitivity limitations that are intrinsic of these samples. The resolution of the protein spectra are outstanding and allow for tracking minimal perturbations that occur in the interaction with the inorganic component^[5] or in response to the presence of ligands.^[6] As a final case study we will discuss an asparaginase-hydroxyapatite composite that is conceived for biocompatible implants for the treatment of acute leukemia: significant structural information can be achieved through NMR about both the enzyme, the material, and their relative.

This work has been supported by Ente Cassa di Risparmio di Firenze; the EU ESFRI Instruct; FIRC 17941 and PhosAgro/Unesco/IUPAC green chemistry for life award.

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Synthesis of CuO/TiO₂ photocatalytic nanocomposites by a modified precipitation approach

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Oral Presentation OP24

Titanium dioxide (TiO₂) is certainly the most used photocatalytic material. It has been known that the addition of a second material, either as metal or metal oxide, yields nanocomposites with better catalytic performance than the pristine one [1]. Among inorganic oxides, CuO is one of the most used for this purpose. The complex-precipitation (CP) technique [2] has been claimed to afford highly dispersed CuO onto TiO₂ surface, improving its photocatalytic activity. Herein we reported a CP synthesis with two different ligands never tested before, namely 1,3-propanediol and citric acid. Moreover, we also prepared a nanocomposite by wetness impregnation, as comparison. Reactivity tests were performed on a lab-made gas-phase photoreforming rig, assessing better activity for CP samples than impregnated one. To understand the reasons of this enhancement of activity, several characterization methods were used. First, temperature programmed reduction (TPR) showed a lower reduction temperature for CP samples, thus suggesting a weaker interaction of CuO with TiO₂ compared to impregnated ones. Second, FTIR analyses displayed a remarkably lower exposition of TiO₂ surface hydroxyl moiety in CP samples, ascribable to a higher dispersion of CuO covering the titanium dioxide surface. In conclusion, we have developed a CP technique using two new ligands, that affords highly-active photocatalytic nanocomposites. This enhanced catalytic activity can be ascribed to weak-interacting and highly-dispersed CuO on TiO₂ surface.

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Flash Oral Presentations

Hydrothermal synthesis of composites of conversion materials and TiO₂ for Li-ion battery anodes

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Flash Oral Presentation FP1

A Continuous Hydrothermal Flow Synthesis (CHFS) process was used to make a range of conversion active materials for Li-ion battery anodes. Conversion materials such as MoO₂ and NiCo₂O₄ are promising anodes in Li-ion batteries because of their high theoretical capacities of 838 and 884 mAh g⁻¹, respectively. However, they typically suffer from poor cycle life due to large volume changes upon lithiation/delithiation, poor high rate performance and large voltage hysteresis.

By co-precipitation of the conversion materials (MoO₂, NiCo₂O₄) with a more chemically and physically stable material (such as TiO₂), both rate performance and cycling stability could be improved. Whilst an electrode using a simple mixture of MoO₂ and TiO₂ showed no improvements, the composite samples, especially those with 20 and 33 mol% TiO₂, showed improved cycling stability and rate performance. Whilst MoO₂ nanoparticles showed a capacity of ca. 50 mAh g⁻¹ at a specific current of 5 A g⁻¹, a composite sample (TiO₂)_{0.2}/(MoO₂)_{0.8} showed a capacity of 165 mAh g⁻¹. Furthermore, the same composite sample showed a remaining capacity of 155 mAh g⁻¹ after 250 cycles at a specific current of 2.5 A g⁻¹, whereas pure MoO₂ showed no remaining capacity.

The improved performance of the conversion materials by co-precipitation with TiO₂ was ascribed to two factors: firstly, the surface areas of the composite were significantly higher than for the pure conversion materials, partly due to a smaller particle size of TiO₂ and partly due to a size reduction to the conversion materials due to more heterogenous nucleation in the synthesis. Secondly, the stability of TiO₂ in the electrode acted as an “anchor” for the reduced metal and for the back-reaction of Li₂O upon delithiation. Because of their higher capacity than most insertion materials, good performance at high rate, and good stability, combinations of conversion materials and stable phases are of interest as potential replacements for graphite anodes in Li-ion batteries.

Exploring the synthesis of zinc sulfide: design and optimisation of new functional nanostructures

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Flash Oral Presentation FP2

ZnS nanostructures are a promising class of material disclosing a wide range of possible applications. ZnS is conveniently used to develop quantum dots for bioimaging applications (as doped) and it is also a known active photocatalyst for the hydrogen evolution reaction (HER). In the literature, a wide range of possible syntheses routes is reported, yielding materials with different morphologies and size and displaying different functional properties. In these framework, having as starting point the paradigms of green chemistry principles and the known details about ZnS formation mechanism, we explored a simple, fast, cheap, room temperature and reproducible water-based synthesis route, based on controlled precipitation approach and on earth-abundant and not toxic precursors, yielding sphalerite-phase ZnS nanostructures as small as 6 nm. The material was tested for HER and it was found to evolve molecular hydrogen at a rate close to $37 \text{ mmol g}^{-1} \text{ h}^{-1}$, a noticeable result which is possibly to be ascribed to the very high specific surface area, determined by N₂ adsorption measurements to be greater than $225 \text{ m}^2/\text{g}$. To achieve the fine tuning of the reaction parameters, and to gain an increased productivity and easier scalability, a microfluidic approach was also developed for the same reaction. The modified mixing of the same precursors solutions employed in the former method led to smaller nanoparticles (5 nm), thus confirming the relevance of the mixing as ruling parameter for this reaction. This method is now being tested to easily synthesize transition metal-doped ZnS and lanthanides-doped ZnS nanostructures for luminescence-based applications, such as in vivo bioimaging.

Sustainable synthesis of readily available metallic ceramics as a new generation of catalyst

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Flash oral Presentation FP3

The synthesis of new functional materials is beneficial for several technological applications, especially for those related to renewable energies. In this respect, one crucial step is to replace scarce and expensive catalysts (e.g. platinum) with more abundant and cost-effective materials. Here, nanomaterials play a fundamental role due to their tunable electronic properties and high surface area.

Within this scenario, our research focuses on the synthesis of catalytically active metallic ceramics (MCs), such as metal nitrides and carbides. MCs possess properties of both ceramics and metals, including good mechanical properties, conductivity and catalytic activity. Some MCs also possess an electronic structure close to that of noble metals and are thus considered promising candidate to replace them in many key catalytic processes^[1].

To use MCs for practical applications, an important step is the synthetic procedure which must involve readily available (i.e. abundant) and sustainable precursors, with relatively low reaction temperature and easy to be scaled up. The final compound should be homogeneous, well-defined in shape, pure and crystalline.

It will be shown that these targets can be achieved by using sol-gel based methods where, by simply changing the N/C source (e.g. urea^[1], chitosan and sugar-based molecules^[2]), it is possible to control composition, size, surface area and morphology of the final material.

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[2] Z. Schnepp, S. C. Wimbush, M. Antonietti and C. Giordano. *Chemistry of Materials*, 2010, **22**, 5340-5344.

Ni(II) square planar complexes and 4,4'-bipyridine based coordination polymers by mechanochemical and solution-based synthesis

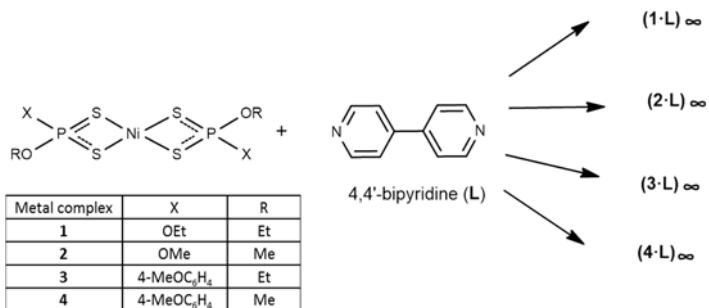
Valentina Cabras^a, Maria Carla Aragoni^a, Simon J. Coles^b, Romina Lai^a, Enrico Podda^a, Martina Pilloni^a, Alessandra Scano^a and Guido Ennas^a

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Flash Oral Presentation FP4

Coordination polymers are technologically important functional materials with noteworthy properties such as porosity, thermo- and photoreactivity. [1] Extending the experience acquired in [2], herein we report the mechanochemical synthesis of the coordination polymers $(2 \cdot L)_{\infty}$, $(3 \cdot L)_{\infty}$, $(4 \cdot L)_{\infty}$ (Scheme 1), obtained by the reactions between the neutral coordinatively unsaturated phosphorodithioato or phosphonodithioato Ni(II) complexes $[Ni((MeO)_2PS_2)_2]$ (**2**), $[Ni(EtOpdt)_2]$ (**3**) and $[Ni(MeOpdt)_2]$ (**4**) ($pdt = (4\text{-MeOC}_6\text{H}_4)\text{PS}_2$) and 4,4'-bipyridine (**L**) as neutral ligand. Several mechanochemical reactions were performed in NG and LAG (with different solvents) approaches. The features of ball milling samples were compared to those of the same samples obtained by solution-based synthesis. The evolution of the reactants during the mechanosynthesis process and the influence of the synthesis parameters on the chemical, structural, and thermal properties of the samples were investigated by XRPD, FTIR, SEM and thermal analysis techniques.



Scheme 1. General scheme of the reaction between complex **1-4** and ligand **L** to give $(1 \cdot L)_{\infty}$ [$(2 \cdot L)_{\infty}$] $(3 \cdot L)_{\infty}$ $(4 \cdot L)_{\infty}$ coordination polymers.

[1] L. R. MacGillivray, *Metal-organic frameworks: design and application*, John Wiley & Sons, **2010**.
[2] V. Cabras, M. Pilloni, A. Scano, R. Lai, M. C. Aragoni, S. J. Coles, G. Ennas, *European Journal of Inorganic Chemistry* **2017**, 2017, 1908-1914.

Ultrasonication of Zn(II) salts and 4,4'-bipyridine for the synthesis of 1D-coordination polymers

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Flash Oral Presentation FP5

In the field of crystal engineering, there is a continuous strong interest in exploring a wide range of synthetic strategies for the preparation of crystalline polymer materials. Ultrasonication is one of the alternative methods for the synthesis of coordination polymers (CPs) and other functional materials (such as Metal-Organic Frameworks, MOFs) with potential applications in catalysis, host-guest chemistry, gas storage/separation, sensors, electrical conductivity and magnetism [1]. Ultrasonication is considered a green synthetic method because of shorter reaction times and higher yields in comparison with conventional synthetic methods [2]. In this work we report the sonochemical preparation of one-dimensional (1D) CPs assembled using 4,4'-bipyridine (4,4'-bpy) as the spacer ligand and chloride or acetate anions, namely $[Zn(4,4'-bpy)Cl_2]$ and $[Zn_2(4,4'-bpy)_2(OAc)_4]_\infty$ respectively. The reactions took place in a very short time (few minutes) compared to conventional methods where some days synthesis are required.

The influence of the synthesis parameters (solvents, temperature) on the chemical, structural, and thermal properties of the samples were investigated by X-Ray Powder Diffraction, Fourier Transform Infrared Spectroscopy, and thermal analysis techniques (Differential Scanning Calorimetry and Thermogravimetry).

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- [2] H. A. A. Tehrani, A. Morsali, *Ultrasonics Sonochemistry* 27 (2015) 503–508

Towards the up-scaled production of highly dispersed ZnO nanoparticles on silica as novel catalyst for the industrial rubber vulcanization process

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Flash Oral Presentation FP6

The mechanical properties of rubber can be highly increased thanks to the vulcanization process, leading to the formation of sulfur cross-linking between polymer chains. To improve the rate and efficiency of this process, several catalysts, including zinc oxide nanoparticles (ZnO NPs) are generally added to the matrix. However, the high hydrophilicity of ZnO hinders a fine distribution of ZnO that tends to agglomerate in the hydrophobic polymer, thus creating non-homogeneous islands of vulcanized rubber and requiring the addition of high zinc content to the matrix. Besides, an environmental issue has been recently connected to zinc release during the life cycle of rubber materials, especially in connection with tyres application.

In this *scenario*, with the aim of reducing the amount of ZnO and improve the vulcanization efficiency, a new vulcanization catalyst has been developed [1], in which ZnO NPs are dispersed onto the surface of silica particles (ZnO/SiO₂); as silica is a common reinforcing agent, the supported catalyst behaves as a “double function filler”. A laboratory scale synthetic procedure has been studied in detail, based on a sol-gel procedure, that allows the formation of amorphous ZnO NPs on silica surface and lead to an improved vulcanization efficiency, with half of the amount of zinc employed. Besides, the production of higher reinforced materials with reduced zinc content was achieved on a preindustrial scale (TRL5). Thus, ZnO/SiO₂ has showed to be a good candidate to substitute the conventional catalyst in the vulcanization process. As a next step, the development of the large-scale production of the material is under examination, in order to get a low-cost production process, maintaining at the same time the initial catalytic properties and to allow its further commercialization.

[1] A. Susanna et al., Chemical Engineering, 2015, 275, 245-252

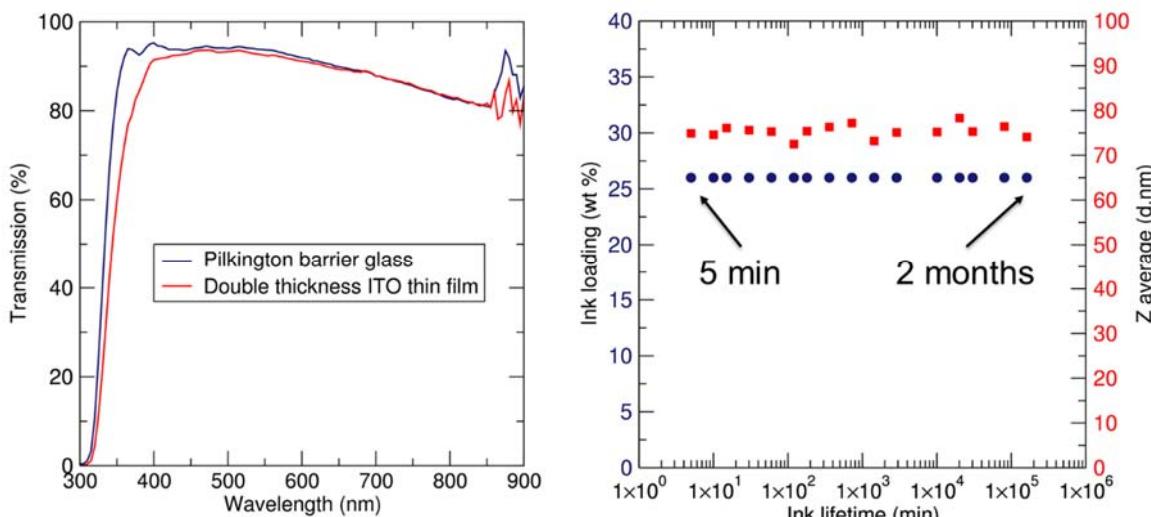
Continuous hydrothermal synthesis of functional nanoceramic inks for printing applications

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Flash Oral Presentation FP7

Functional thin films are widely used in a variety of applications including mobile phones (transparent conducting oxides; TCOs), smart windows (thermochromics) and solar cells. Deposition techniques for the generation of such films commonly takes place using wide area techniques, with little control over fine area resolution such as screen printing and chemical vapour deposition. Even if the spatial resolution can be achieved by masking, this is an inherently wasteful process. The spatial resolution of the deposition techniques is increasingly important with the rise of next generation electronic devices.



To combat these issues, we have developed functional indium tin oxide (ITO) nanoparticle inks for TCO applications using a scalable, continuous hydrothermal flow synthesis (CHFS) method on a 2 Kg h⁻¹ scale. This has been achieved by a two-step in-flow process, whereby (i) nanoparticles are precipitated from their respective salts and (ii) the nanoparticles are subsequently coated with a surfactant. It has also been demonstrated that these coated nanoparticles are stable in a wide pH range and remain suspended indefinitely. A suitable vehicle for inkjet printing has also been identified, and various deposition have been successfully carried out with resistances in the order of 10^{-3} Ω cm, and optical transparencies exceeding 85 %.

On the physico-chemical properties of a novel class of saponite clays containing lanthanide ions in framework position

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Flash Oral Presentation FP8

Synthetic saponite clays have stimulated particular interest over the past few decades due to their interesting properties, such as high thermal stability and excellent chemical versatility. The introduction of *f*-block elements (*i.e.* ions or complexes) in the clay framework may lead to a new class of materials with novel electronic, magnetic, optical or catalytic properties. Thus, in this work we synthesized a saponite clay with both Gd³⁺ and Eu³⁺ ions into the inorganic framework, through a modified hydrothermal method, obtaining a material with both magnetic and luminescent properties (Na-GdEuSAP). Samples containing only Gd³⁺ or Eu³⁺ ions have been also prepared as references (Na-GdSAP, Na-EuSAP). The Gd³⁺ and Eu³⁺ loading resulted to be 0.02 mmol/g and no concentration reduction was detected after the Na⁺-exchange procedure, thus suggesting that the lanthanides are mainly located in framework positions. The presence of these ions did not alter the crystalline structure of saponite samples, as observed by XRD analyses. SEM and TEM microscopy analyses indicated that the samples present different levels of spatial organization of lamellae, with a size of few tens nanometers. The photophysical properties of samples were studied by photoluminescence spectroscopy. The luminescence spectrum showed the characteristic peaks of the Eu³⁺ and the presence of Gd³⁺→Eu³⁺ energy transfer process was proved. The average hydration of the Eu³⁺ (*q*), estimated through the analysis of the radiative lifetimes (τ) in H₂O and in D₂O, was *ca.* 4. The intrinsic quantum efficiency of Eu³⁺ ($\Phi^{\text{Eu}_{\text{Eu}}}$) was established to be 4.29%. A complete ¹H NMR relaxometric study was then performed on samples. ¹H 1/T₁ NMRD profiles show the typical shape of slowly tumbling systems, with a broad hump centered at *ca.* 0.4 Tesla. Samples showed improved relaxometric performances at high magnetic fields as compared to commercial Gd³⁺-chelates. Gd³⁺ release tests, performed in the presence of EDTA ligand, confirmed the high chemical stability of materials, with absence of Gd³⁺ and Eu³⁺ leaching.

Highly dynamic and tunable behavior of 1D coordination polymers based on the bispidine ligand

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^aDepartment of Chemistry, Materials and Chemical Engineering, Politecnico di Milano.

Flash Oral Presentation FP9

Coordination polymers (CPs) are class of new hybrid materials that have recently attracted enormous interest due to their wide field of possible applications such as storage, separation and catalysis.¹ Particular attention has been devoted to dynamic coordination polymers, belonging to the 3nd generation compounds in Kitagawa's classification² which are able to change their physical and chemical behavior in response to external stimuli.

Bispidines are a class of robust and versatile organic ligands commonly employed for metal binding but, to our surprise, never used for building coordination polymers.

In this work, we have designed and synthesized two bispidine ligands **1** and **2** (Figure 1a), which have been then used to obtain CPs in combination with Mn(II) ions.

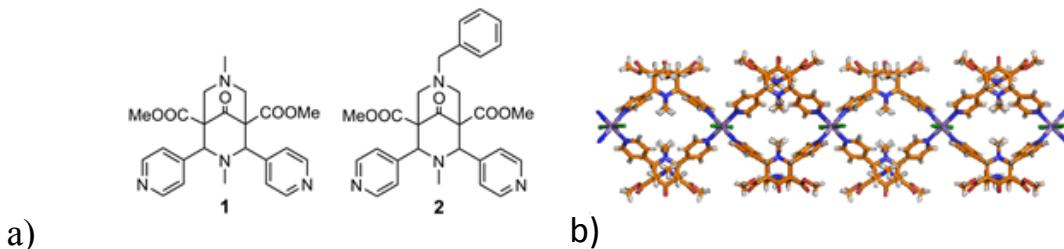


Figure 1. a) Molecular formulae of bispidine derivatives **1** and **2**. b) 1D ribbons of repeating complex units.

We obtained and characterized by SC-XRD six novel Mn(II) 1D CPs which feature linear 1D ribbon-like structures of repeating 2:1 ligand:metal complex units (Figure 1b). We were also able to produce and characterize several microcrystalline phases, which we then used to test heterogeneous solid/liquid and solid/gas solvent exchange processes. We found out that these materials possess a unique and highly dynamic behavior as they can undergo several types of transformations, comprising less common crystalline-to-amorphous-to-crystalline, non-porous to porous, and selective solvent adsorption processes. Most importantly, CPs made with **1** show different response than those made with **2**, indicating that by simply modulating the inter-ribbon interactions the response of the CPs in terms of heterogeneous guest exchange can be efficiently controlled.

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Continuous hydrothermal synthesis of perovskite titanates for use as oxygen reduction catalysts

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Flash Oral Presentation FP10

Electrochemical reduction (ORR) and oxidation of water (OER) are important reactions for a variety of applications including fuel cells, metal air batteries and energy storage devices. However, electrode kinetics are sluggish and require the use of electro-catalysts to make reactions commercially competitive. These catalysts are traditionally precious metals such as platinum and iridium which are expensive and scarce. Perovskite based catalysts have an advantage over traditional precious metal catalysts as they are cheaper, more thermally and chemically stable and lighter. The intrinsic activity of perovskites for the oxygen reduction reaction is close to iridium making families of this structure an interesting area of study.

We have successfully synthesised a ternary library of 66 titanate materials with the ABO_3 perovskite structure where A is a combination of barium, strontium and calcium and B is titanium. These were synthesised using a continuous hydrothermal flow reactor where dissolved precursors meet a stream of supercritical water in flow, rapidly precipitating nanoparticles. These have been tested for their activity for the oxygen reduction reaction using a rotating disk electrode showing competitive catalytic behaviour, which is sensitive to the elemental composition.

Poster Presentations

Polymorphic synthesis of porous zeolites monoliths

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Poster Presentation P1

Zeolites are suitable materials for several processes such as catalysis, adsorption, separation etc. However, their porous structure results in low diffusion and reaction rates, which is a strong restriction to their use in industrial applications [1]. To overtake these limitations, recent studies focused on the synthesis of hierarchically meso/microporous or macro/microporous zeolitic monoliths, in which relatively larger cavities, such as meso- or macropores, are present together with the characteristic zeolitic micropores.

In this work, such monoliths have been produced via hydrothermal treatments on porous silica monoliths, used as a structural support as well as a silica source. This process can be considered as a pseudomorphic transformation, in which the dissolution rate of the silica precursor is controlled and adapted to the rate of formation or crystallization of the zeolite to preserve the morphology of the parent silica material. In a typical experiment, silica monoliths samples are prepared starting from TEOS, water and PEO [2], and then impregnated with a solution of silica fumed, TPAOH, NaOH, water and NaAlO₂. Samples are then put in an autoclave at a certain temperature for a sufficient amount of time. Depending on treatment time, temperature, impregnating solution composition and silica monolith amount, different types of zeolites can grow. In this work, zeolites such as NaP1, LTA and NaP1/NaLTA/NaFAU aggregates have been obtained, and characterized by X-Ray diffraction.

[1] Tokudome Y., Nakanishi K., Kosaka S., Kariya A., Kaji H., Hanada T. (2010) Synthesis of high-silica and low-silica zeolite monoliths with trimodal pores. *Microporous and Mesoporous Materials* 132, 538–542.

[2] Said B., Cacciaguerra T., Tancré F., Fajula F., Galarneau A. (2016) Size control of self-supported LTA zeolite nanoparticles monoliths. *Microporous and Mesoporous Materials* 227 176-190

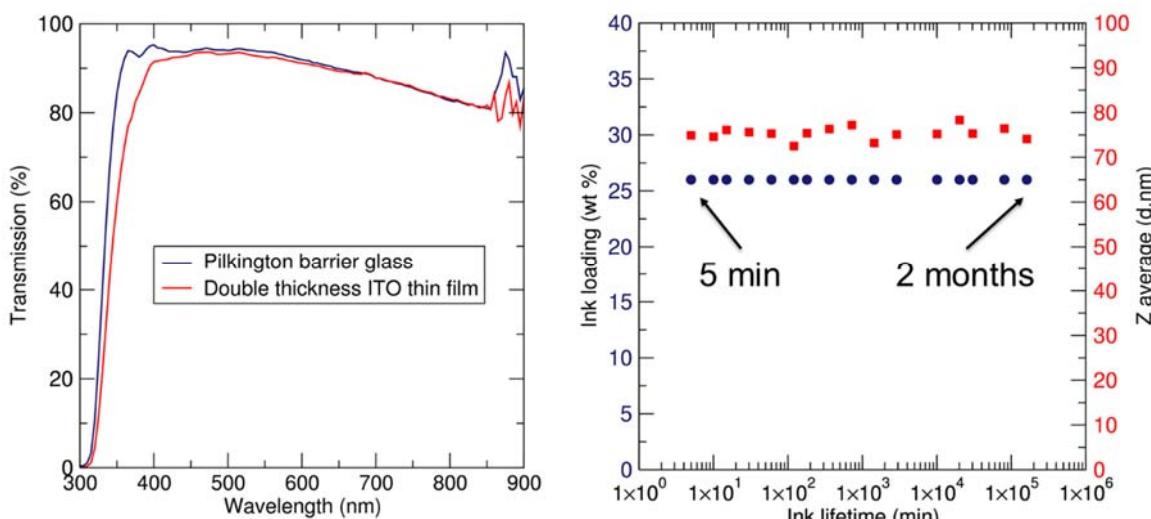
Continuous hydrothermal synthesis of functional nanoceramic inks for printing applications

Thomas E. Ashton^a, Carlos Sotelo-Vazquez^a and Jawwad A. Darr^a

^aSchool of Chemistry, University College London, WC1E 0AJ, London, United Kingdom

Poster Presentation P2

Functional thin films are widely used in a variety of applications including mobile phones (transparent conducting oxides; TCOs), smart windows (thermochromics) and solar cells. Deposition techniques for the generation of such films commonly takes place using wide area techniques, with little control over fine area resolution such as screen printing and chemical vapour deposition. Even if the spatial resolution can be achieved by masking, this is an inherently wasteful process. The spatial resolution of the deposition techniques is increasingly important with the rise of next generation electronic devices.



To combat these issues, we have developed functional indium tin oxide (ITO) nanoparticle inks for TCO applications using a scalable, continuous hydrothermal flow synthesis (CHFS) method on a 2 Kg h⁻¹ scale. This has been achieved by a two-step in-flow process, whereby (i) nanoparticles are precipitated from their respective salts and (ii) the nanoparticles are subsequently coated with a surfactant. It has also been demonstrated that these coated nanoparticles are stable in a wide pH range and remain suspended indefinitely. A suitable vehicle for inkjet printing has also been identified, and various deposition have been successfully carried out with resistances in the order of 10^{-3} Ω cm, and optical transparencies exceeding 85 %.

Doped anatase nanoparticles for anodes in Li-ion and Na-ion hybrid electrochemical capacitors

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Poster Presentation P3

A Continuous Hydrothermal Flow Synthesis (CHFS) process was used to make a range of doped TiO_2 (anatase) samples for Li/Na-ion anodes. Nano-sized TiO_2 has been shown to exhibit excellent performance at high rates because of increased pseudocapacitive contributions to charge storage. With CHFS, doped nano-sized TiO_2 (ca. 5 nm) could be synthesised with consistent physical properties, which allowed for excellent comparability between samples. Doping with Mo(VI), V(V), and Nb(V) was expected to improve the electronic conductivity of Mo-, V-, or Nb-doped TiO_2 compared to undoped TiO_2 , which has a large band gap of 3.2 eV, by introducing induced conduction band electrons.

The doping not only increase electrical conductivity, but also the pseudocapacitive charge storage contributions. This resulted in significantly better specific capacities at higher applied specific currents for all doped samples, both in Li-ion and Na-ion half-cells. In Li-ion half-cells, $\text{Mo}_{0.1}\text{Ti}_{0.9}\text{O}_2$, $\text{V}_{0.2}\text{Ti}_{0.8}\text{O}_2$, and $\text{Nb}_{0.25}\text{Ti}_{0.75}\text{O}_2$ showed specific capacities of 40, 40, 50 mAh g⁻¹, respectively, higher than the 25 mAh g⁻¹ for TiO_2 . In Na-ion half-cells, $\text{Mo}_{0.1}\text{Ti}_{0.9}\text{O}_2$, $\text{V}_{0.2}\text{Ti}_{0.8}\text{O}_2$, and $\text{Nb}_{0.25}\text{Ti}_{0.75}\text{O}_2$ showed specific capacities of 45, 50, and 45 mAh g⁻¹, compared to just 15 mAh g⁻¹ for TiO_2 , at a specific current of 2.0 A g⁻¹.

Li/Na-ion Hybrid Electrochemical Capacitors (HECs), which employ a combination of EDLC electrodes (high surface area carbons) and battery-type electrodes (anatase TiO_2), can bridge the gap between high-energy batteries and high-power capacitors. In contrast to batteries, in HECs, symmetrical driving forces lead to the migration of cations and anions to opposite electrodes during charge/discharge. Because of the high pseudocapacitive charge storage contributions for the doped samples, they exhibited excellent performance in Li/Na-HECs, whereas pure TiO_2 showed worse performance. A pre-sodiated $\text{Mo}_{0.1}\text{Ti}_{0.9}\text{O}_2/\text{AC}$ Na-HEC showed energy densities of 80, 73, and 42 Wh kg⁻¹, at power densities of 280, 570, and 2630 W kg⁻¹, respectively. In comparison, a non-pre-sodiated TiO_2/AC Na-HEC showed an energy density of 35 Wh kg⁻¹ at a power density of just 300 W kg⁻¹.

**Low-temperature crystallization of solution-derived metal oxide thin films assisted by
photochemical processes**

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Poster Presentation P4

The versatility of wet chemical methods allows the exploration of novel crystallization pathways for metal oxides thin films and makes them fundamental in the search of low-temperature methods. The benefits obtained from decreasing the processing temperature span from minimizing the environmental impact to reducing the production costs. More challenging is the preparation of complex oxide layers at temperatures compatible with their direct integration in flexible substrates (≤ 350 °C). However, their high crystallization temperatures (>600 °C) impede the development of such multifunctional devices. Significant efforts have been devoted in our group to address this challenge [1]. The result is an efficient series of strategies for the low-temperature processing of oxide layers using light as an alternative energy source to induce crystallization by photochemistry. Here, it will be shown how the crystallization of photoferroic BiFeO₃, ferroelectric Pb(Zr,Ti)O₃ or photocatalytic β -Bi₂O₃ can be achieved at temperatures between 250-350 °C. This requires the synthesis of novel photosensitive solutions (modified metal alkoxides, charge-transfer metal complexes, structurally designed molecular compounds) and precise control over the reactions promoted by UV light (photochemical cleavage, ozonolysis, condensation, photocatalysis).

[1] I. Bretos, R. Jiménez, J. Ricote, and M.L. Calzada, *Chem. Soc. Rev.*, 2018, **47**, 291-308

**Microwave reactors for hydro- and solvothermal synthesis. Optimal performances,
measurements problems and scale up possibility**

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Poster Presentation P5

Microwave solvothermal synthesis (MSS) is the great example of microwave assisted wet chemical synthesis process. In today's world it is counted as one of the most popular chemical methods of obtaining nanopowders, like HAP, ZnO, ZrO₂, doped materials and other. Microwave heating enables a better control of the reaction time, fast heating and reducing the thermal gradients. The morphology, grain size and specific surface area of the nanopowder can be controlled by the microwave reactor and the high pressure consolidation technology for ceramic materials, this also results in a better crystallinity comparing to the precipitation process.

At the Laboratory of Nanostructures, IHPP PAS, we have been developing new type microwave reactors for nanomaterials synthesis for more than 10 years. The use of the microwave radiation and the unique design of the reactor permit precise pressure control during the quick synthesis processes, controlled with the accuracy of even one second. The reactor also presents a control system which allows for an automatic operation in the stop flow mode or use the batch (closed vessel) mode in bigger production scale than in other commercial equipment. [1] Temperature measurements of the suspension are quite difficult, thermocouples can be burned out by sparking and also generate errors, strongly absorbing materials inside the reactor can also misjudge the IR sensor and showing not reliable temperature. Better way in that situation (ionic liquids inside) is using fiber-optic sensors, which are in contact with reaction mixture.

[1] A. Majcher, J. Wiejak and et al. Int. J. Chem. Reactor Engineering 2013, 11, 361-368

Design and realization of photocatalytic coatings based on TiO₂ nanoparticles

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Poster Presentation P6

TiO₂ nanoparticles (NPs) with their excellent photocatalytic performance are among the most investigated materials for environmental clean-up applications.^[1] The present work investigates the impact on the photocatalytic activity, of two different deposition techniques designed to be suited for a scalable production TiO₂ NPs coating onto different possible substrates, namely, the *doctor blade* technique and a purposely developed *dip coating* method, here defined as *inverted dip coating*. To this end, a batch of TiO₂ NPs was synthesized by slightly modifying a reported approach, specifically selected for its scalability.^[2] The obtained product was characterized by X-ray diffraction analysis, TEM microscopy and diffuse reflectance spectroscopy and successively deposited by using the two proposed approaches onto glass slides, used as a model support. In particular, the TiO₂ coatings were deposited by means of the *doctor blade* technique and the *inverted dip coating* method, from isopropanol suspensions of TiO₂ NPs, at a concentration of 6,5%, 13% and 26% by weight, respectively. After investigating the morphology of the obtained TiO₂ NPs based coatings, their photocatalytic activity was assessed by monitoring the decolouration of a dye, the Methylene Blue (MB) in aqueous solution under UV light irradiation, and the adsorption of dye was tested, as well. Experimental results revealed that, regardless the deposition technique, the TiO₂ NPs based coating prepared from the 13% TiO₂ NP suspension demonstrated the most effective in MB photodegradation, under the applied experimental conditions. The reported results are very promising for the investigation of efficient, convenient and scalable approaches for preparation of photocatalytic coating based on TiO₂ NPs for their sustainable application in environmental technologies.

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Synthesis of quaternary spinel ferrites via continuous flow and conventional autogenous hydrothermal synthesis

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Poster Presentation P7

Spinel ferrites having general formula MFe_2O_4 are extremely useful and versatile inorganic materials, with numerous functional properties ranging from magnetic, to dielectric, to catalytic and beyond which allow them to find application in a wide array of fields [1]. Within this class of materials, ternary spinel ferrites (a subset of spinel ferrites, also known as mixed ferrites, containing two M metals and having chemical formula $M_xM'_{1-x}Fe_2O_4$) arise particular interest, as the presence of two metal species (having different electronic configuration) within the same spinel lattice can give rise to several interesting properties [2]. We report the synthesis of the ternary ferrites $Co_xZn_{1-x}Fe_2O_4$ and $Ni_xZn_{1-x}Fe_2O_4$ ($X = 0, 0.2, 0.35, 0.5, 0.65, 0.8, 1$) though a low-temperature conventional hydrothermal (HT) synthesis protocol (adapted from a previous work) [3] as well as through continuous flow hydrothermal synthesis (CFHS) [4]. The materials resulting from the two synthetic approaches were thoroughly characterised from a structural (XRD) and compositional (XPS, ICP-MS) point of view and the results were evaluated in order to achieve a good comparison between batch and CF hydrothermal approaches.

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[2] Mohan, R.; Ghosh, M. P.; Mukherjee, S. *J. Magn. Magn. Mater.* **2018**, 458, 193-199

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Method to the magic; materials discovery of magnetic and dielectric nanoparticles for medical application

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Poster Presentation P8

Continuous flow hydrothermal synthesis (CHFS) is a scalable and sustainable route towards the rapid synthesis of nanomaterials, applicable to a diverse range of applications. Metal salts are intimately mixed with supercritical water ($T > 374\text{ }^{\circ}\text{C}$, $P > 22\text{ MPa}$) in a patented confined jet mixer, inducing instantaneous heating and mixing of the two fluids at the mixing point such that the solubility of the metal source decreases, and the nucleation of nanoparticles (oxides, titanates, ferrites, metals) ensues. Reaction times are $< 5\text{ s}$ and nucleation and growth processes can be controlled and manipulated by varying process parameters. This novel and exciting technique has been employed in this project as the foundation for a materials discovery methodology which has its foundations in pharmaceutical companies' drug discovery efforts and explores the capabilities of QinetiQ and UCL in order to discover interesting and novel candidates for use in electromagnetic applications such as that in remedial healthcare and treatment of illnesses such as cancer. This ambitious project involves the employment of a variety of different fields of science including: materials synthesis; process engineering; chemical characterisation; physical testing; mass data collection and storage; data mining; and macro analysis. This methodology and its associated work mean that a new level of understanding can be developed of the relationship between structure and electromagnetic response. The first 18 months of this PhD programme have been successful in synthesising and electromagnetically characterising over 700 nanoparticle candidates.

Oxygenic activity of multinuclear manganese complexes

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Poster Presentation P9

Manganese-complexes answer to the need of using abundant and biocompatible metals to develop biomimetic catalysts. Mn is indeed present in different oxygenic enzymes, including the photosystem II, superoxide dismutase and catalase [1]. Herein we report two uses of two known Mn oxoclusters [2]: $[\text{CeMn}_6\text{O}_9(\text{O}_2\text{CMe})_9(\text{NO}_3)(\text{H}_2\text{O})_2]$ (Mn_6) and $[\text{Mn}^{\text{III}}_2\text{Mn}^{\text{II}}_6\text{O}_2(\text{PhCOO})_{10}(\text{dmhmp})_4(\text{H}_2\text{O})_2$ (Mn_8), (Figure 1). The first is a hexanuclear Mn oxocluster stabilized by peripheral carboxylates and by a templating Ce core, while the second is a neutral compound with eight Mn atoms protected by four dmhmp ligands and ten PhCOO ligands. Another strategy to develop Mn complexes is offered by the possibility to incorporate a polynuclear Mn core into a polyoxometalate (POM) [3]. To this aim, a tetranuclear rhomb-like cluster of Mn(II) was assembled between two trivacant tungstophosphate ligands [4] $[\alpha\text{-PW}_9\text{O}_{34}]^{9-}$ and $[\text{P}_2\text{W}_{15}\text{O}_{56}]^{12-}$ to yield $\text{K}_{10}[\text{Mn}_4(\text{H}_2\text{O})_2(\text{PW}_9\text{O}_{34})_2]$ and $\text{Na}_{16}[\text{Mn}_4(\text{H}_2\text{O})_2(\text{P}_2\text{W}_{15}\text{O}_{56})_2] \cdot 53\text{H}_2\text{O}$, respectively (Figure 1).

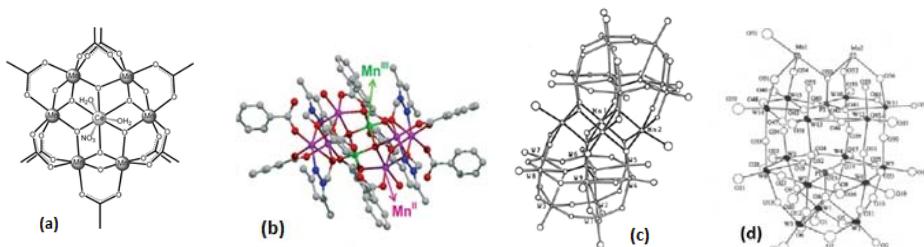


Figure 1.

The catalytic activity of these complexes was tested towards H_2O_2 dismutation into H_2O and O_2 . The evolution of O_2 was monitored at pH 7, by a differential pressure transducer: the most effective is Mn_6 , for which the activity remained constant during the monitoring, reaching the complete conversion of H_2O_2 after 12h, with a turnover number (TON) >800 .

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Copper vanadate photoanodes prepared by aerosol assisted atmospheric pressure cold plasma jet

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Poster Presentation P10

Copper vanadate are an interesting class of transition metal oxide that are considered very promising materials for the preparation of photoanodes in water splitting devices, thanks to the ideal amplitude of their band gap (ca. 2 eV) and valence band edge position. Nevertheless, there are some drawbacks like the corrosion of vanadium (as vanadium oxyanion) and the short diffusion length of photo-generated holes [1]. These characteristics can be tuned and optimized by changing the ratio between Cu and V. Usually, a high concentration of copper prevents the degradation of the material thanks to a passivating film of CuO_x, but at the same time the performances worsen due to the presence of surface trap states (Cu²⁺ center)[1]. So we decided to study a phase that is a compromise between durability and efficiency. The ziesite (β -Cu₂V₂O₇) is characterized by a band gap of 1.98 eV and the position of conduction band is at about 0.7 V vs RHE [2]. These characteristics allow a good solar light absorption and a good positioning of valence band edge for water oxidation.

The deposition of this material was performed, for the first time, using a very convenient atmospheric pressure plasma jet, starting from a simple precursor solution (ammonium vanadate, malachite and citric acid). This type of experimental setup also allows to obtain the deposition of complex patterns on any type of support thanks to a motorized x-y stage. The Plasma partially decomposes the ligand in the precursor solution droplets so that the copper vanadate starts to nucleate already in the aerosol’s drop. The result is a deposit characterized by nanorods-shaped particles organized in a macro porous network.

The deposits were characterized by SEM, XPS, XRD, Raman and EC measurements.

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- [1] Sharp, I. D. et al. Composition-Dependent Functionality of Copper Vanadate Photoanodes. *ACS Appl. Mater. Interfaces* **2018**, acsami.8b02977.
 - [2] Mullins, C. B. et al. Synthesis and Characterization of CuV₂O₆ and Cu₂V₂O₇: Two Photoanode Candidates for Photoelectrochemical Water Oxidation. *J. Phys. Chem. C* **2015**, 119, 27220–27227.

Continuous hydrothermal synthesis of perovskite titanates for use as oxygen reduction catalysts

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Poster Presentation P11

Electrochemical reduction (ORR) and oxidation of water (OER) are important reactions for a variety of applications including fuel cells, metal air batteries and energy storage devices. However, electrode kinetics are sluggish and require the use of electro-catalysts to make reactions commercially competitive. These catalysts are traditionally precious metals such as platinum and iridium which are expensive and scarce. Perovskite based catalysts have an advantage over traditional precious metal catalysts as they are cheaper, more thermally and chemically stable and lighter. The intrinsic activity of perovskites for the oxygen reduction reaction is close to iridium making families of this structure an interesting area of study.

We have successfully synthesised a ternary library of 66 titanate materials with the ABO_3 perovskite structure where A is a combination of barium, strontium and calcium and B is titanium. These were synthesised using a continuous hydrothermal flow reactor where dissolved precursors meet a stream of supercritical water in flow, rapidly precipitating nanoparticles. These have been tested for their activity for the oxygen reduction reaction using a rotating disk electrode showing competitive catalytic behaviour, which is sensitive to the elemental composition.

Sustainable saccharide templates to drive the formation of hierarchical SAPO-34 with tunable acid properties

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Poster Presentation P12

Hierarchical zeolites or zeotype materials, which combine both micro and mesopores in a multilevel pore network, strongly emerged as novel materials for catalytic applications to overcome typical drawbacks of traditional microporous materials such as poor mass transfer and hindered diffusion. A wide variety of innovative strategies to produce secondary porosity within the framework of microcrystalline structures has been developed, nevertheless, significant challenges are still ahead. In a novel and distinct bottom-up approach, monosaccharides and disaccharides have been used along with the micropore SDA to template hierarchical SAPO-34 catalysts¹. Structural and textural properties of the hierarchical materials were evaluated by means of powder XRD and volumetric analyses. In addition, to get information on the nature, strength and the accessibility of the acid sites in the hierarchical catalysts, a fine physico-chemical characterization using FT-IR spectroscopy of adsorbed probe molecules together with solid-state NMR was also performed. The hierarchical SAPO-34 catalysts showed superior activity in the Beckmann rearrangement of cyclohexanone oxime to ϵ -caprolactam (precursor for Nylon-6) with respect to the parent microporous systems, thanks to the overcoming of the diffusion constraints due to the introduction of mesoporosity.

[1] Miletto, I.; Ivaldi, C.; Paul, G.; Chapman, S.; Marchese, L.; Raja, R.; Gianotti, E. *ChemistryOpen* **2018** 7:297-301
The project leading to these results has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement N. 720783—MULTI2HYCAT

Microwave assisted hydrothermal synthesis of luminescent doped fluoride materials

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Poster Presentation P13

Lanthanide and transition metal doped luminescent nano and micromaterial are a interesting topic for many scientific and technological fields such as optical bioimaging, nanothermometry, upconversion emission for photovoltaic or photocatalytic reaction.

Microwave-assisted hydrothermal synthesis is an appropriate technique for study these materials: it allows fast and homogeneous heating, short reaction time, high reproducibility and ease of scale up for industrial synthesis. The faster heating and shorter reaction time, compared with normal hydrothermal reactors, allows to prepare many more samples and properly study the parameter that influence the synthesis.

In this contribution we will report the microwave-assisted hydrothermal synthesis of some doped fluoride materials and how reaction parameters (such as reagent concentration, dopant concentration, reaction time, temperature etc.) can modify the propriety of products (such as morphology, size, luminescence).

Metal–organic coordination networks of tetrahydroxyquinone on Cu(111) based on copper adatom tetramers

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Poster Presentation P14

In the last few years, coordination chemistry has been widely exploited to organize secondary building units (SBUs) into well-ordered nanostructures [1]. Besides basic research, metal–organic coordination networks (MOCNs) and surface-supported MOCNs have diverse technological applications ranging from molecular recognition to catalysis, gas storage and separation [2].

In this study, scanning tunneling microscopy (STM) measurements have been combined with periodic DFT calculations to investigate the synthesis of a surface supported coordination network obtained from tetrahydroxyquinone (THQ) SBUs on Cu(111) surface. Numerical experiments have been performed with and without the inclusion of dispersion corrections. The results confirm and further refine the previously proposed model [3]: the preferred configuration for THQ molecules on Cu(111) under annealing up to ~ 385 K corresponds to a dehydrogenated molecule (TOQ) directly bound to tetrameric Cu adatoms (occupying hollow positions) through oxygen atoms with the phenyl ring center positioned on a top site (see Figure 1(b)). The inclusion of the long-range dispersion forces provided a very good agreement between the experimental STM image (Figures 1(a)) and its simulation (Figure 1(c)).

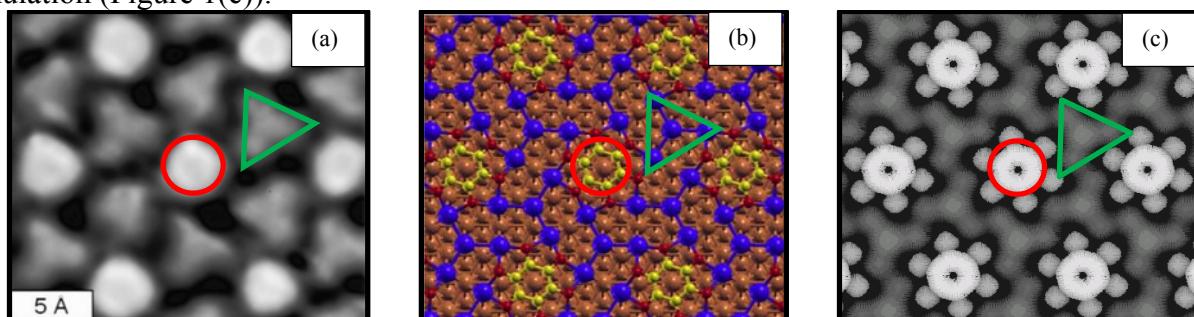


Figure 1 Top views of (a) experimental STM image, (b) corresponding DFT-optimized geometry and (c) simulated STM image of the TOQ molecule assembled on the Cu(111) surface at ~ 385 K and a bias voltage of $V = 0.55$ V.

[1] Dürren T., Bae Y. S., Snurr R. Q., *Chem. Soc. Rev.*, 2009, **38**, 1237.

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Unconventional hierarchically porous niobium-titanium oxide monoliths for the catalytic dehydration of xylose to furfural under continuous flow

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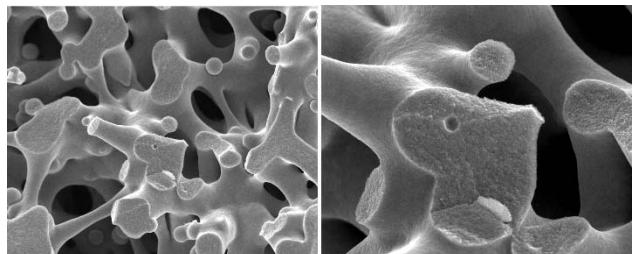
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Poster Presentation P15

The approach herein pursued is the synthesis of unconventional solid acid monolithic catalysts based on a mixed niobia-titania skeleton building up a hierarchical open-cell network of mesopores ($2 < x < 50\text{ nm}$), what allows efficient processing, and macropores ($x > 50\text{ nm}$) with benefits in terms of reduced pore clogging, better active sites accessibility and improved mass transfer.

The materials were characterized by spectroscopic, microscopy and diffraction techniques showing a reproducible, isotropic structure and an increasing Lewis / Brønsted acid sites ratio with increasing Nb content. Application of the synthesized monoliths in the development of sustainable methods for biomass valorization was tested through a reaction of great relevance; the acid-catalyzed dehydration of xylose to furfural. The efficiency of the catalyst showed to be dramatically affected by the niobia content in the titania lattice. The presence of as low as 2% wt niobium resulted in a furfural yield of 39% at 140 °C reaction temperature and 224 s residence time under continuous flow conditions, using H₂O / γ-valerolactone as safe monophasic solvent system. The interception of a transient 2,5-anhydroxylose species suggested the dehydration process to occur via a cyclic intermediates mechanism. The catalytic activity and the formation of the anhydro intermediate were related to the LAS/BAS ratio and indicated a significant contribution of xylose-xylulose isomerization. No significant catalyst deactivation was observed over 4 days' usage.



Typical SEM images of NbTiO-MNL2

[1] [N. Linares, S. Hartmann, A. Galarneau, P. Barbaro, ACS Catal. **2012**, 2, 2194-2198]

Pro-osteogenic mesoporous glasses with zwitterionic surface for bone regeneration

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Poster Presentation P16

Since 2004, Mesoporous Bioactive Glasses (MBGs) have been considered a promising system to improve bone regeneration [1], due to their superior *in vitro* bioactivity combined with the ability to act as drug delivery system. Nonetheless, a severe limit to the treatment of bone defect is represented by the occurrence of bacterial infections. Therefore, the development of pro-osteogenic biomaterials able to stimulate bone tissue regeneration and, simultaneously, inhibit bacterial adhesion is gaining increasing interest.

In this context, zwitterionisation [2], which involves the functionalization with an equal number of surface positively and negatively charged moieties, is a promising strategy to provide MBGs with bacterial anti-adhesive properties.

In this study, SiO₂-CaO based MBGs containing therapeutic ions (Sr²⁺, Cu²⁺) were synthesized in the form of micro- and nanoparticles. In order to provide them with the ability to prevent bacterial adhesion, zwitterionisation procedures were performed. Specifically, grafting of primary/secondary amines and amino acid molecules to the surface -OH groups was carried out and the resulting zwitterionic MBGs were loaded with drugs.

Samples were characterized through EDS, FE-SEM, N₂ adsorption-desorption measurements, TGA, FT-IR, DLS, zeta potential and elemental chemical analysis to confirm both the anchoring of zwitterionic groups and the drug loading. Moreover, the release of therapeutic ions and drugs and *in vitro* bioactivity were evaluated.

[1] Xiaoxia Yan *et al.*, Angew. Chem. Int. Ed. 43, (2004), 5980-5984.

[2] Isabel Izquierdo-Barba *et. al*, Acta Biomaterialia 40, (2016), 201–211.

Crystal phase controlled synthesis of TiO₂ nanoparticles by solution combustion method

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Poster Presentation P17

Nanostructured materials are in great demand for environmental and energy-related applications. The combustion synthesis (CS) or self-propagating high-temperature synthesis (SHS) is a competent fast and energy saving method for the synthesis of nano-materials for different needs. The aqueous solution reaction media, high reaction temperature and short process duration are the advantages of CS. These advantages allow engineering of materials with desired composition at nanoscale, provide products purity and crystallinity, and favor production of nanosized powders with high specific surface area. The possibility to control crystal phase parameters during synthesis is one of the basic steps for achieving highly efficient materials. In the case of TiO₂ the possibility to control formation of anatase and rutile phases or their mixture gives an opportunity to design nanoparticles with properties meeting the required demands. Toward this direction, we successfully prepared TiO₂ powders with diverse crystal phase compositions in a controllable fashion by solution combustion synthesis. The titanium oxynitrate (TiO(NO₃)₂) prepared from titanium tetrachloride (TiCl₄≥99,90%) and carbohydrazide (CO(N₂H₃)₂ 97%) were used as a TiO₂ precursor and fuel, respectively. It was found that the crystal phase of the TiO₂ particles can be easily tuned by varying the external conditions such as chloride and fluoride ions concentration in the starting solution. As sources of chloride and fluoride ions hydrochloric (HCl, 32%) and hydrofluoric (HF, 40%) acids were used. Series nanopowders including rutile, anatase and their mixtures in different ratios, had been synthesized to demonstrate the versatility of our strategy. Nanopowders photocatalytic activity was tested by Reactive blue 19 (RB19) degradation rates. Results showed that the ability of synthesized TiO₂ powders to decompose RB19 is dependent of crystal phase of obtained powders and in case of mixture phase composition it is comparable with TiO₂ Aeroxide Degussa P25 benchmark photocatalyst.

Mesostructured LaCoO₃ prepared by acrylic polymers for heterogeneous catalysis

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Poster Presentation P18

Ternary oxides like the perovskite oxide LaCoO₃ present a promising alternative to expensive and scarce noble metals (e.g., Pt, Pd) in the field of heterogeneous catalysis. A common way to synthesize these oxide materials is the employment of a polymer complex route, namely the Pechini method. This method is based on citric acid acting as a complexing agent towards the metal cations while also forming a polymer network in combination with an adequate solvent. However, the resulting metal oxides usually contain impurities and the slow polymerization reaction inhibits nanostructuring and therefore the improvement of the textural properties of the material.

In our work, we developed a variation of the polymer complex route, which relies on the use of acrylates (methacrylic acid, acrylic acid, acrylamide) as complexing agents. This novel synthesis provides phase pure perovskite oxides with higher catalytic activity.

In order to assess the impact of the synthesis route on the catalytic activity, the CO oxidation over LaCoO₃ powders synthesized from acrylic complexing agents and from citric acid was compared. As seen in Fig. 1, the acrylic acid and acrylamide based LaCoO₃ display a significantly higher conversion than the LaCoO₃ produced from citric acid. As XPS spectra indicate, this is due to a higher amount of active oxygen species on the metal oxide surface. In addition to a superior catalytic performance, using acrylates as complexing agents facilitates the nanostructuring of the material. As an example, perovskite thin films could be prepared exploiting the radical polymerization induced by UV light.

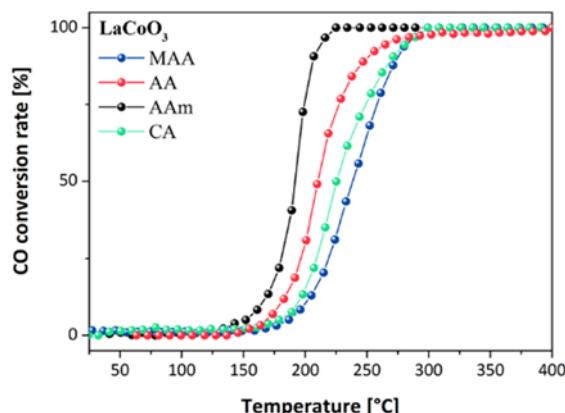


Fig. 1: Conversion rate of CO in dependence of the temperature in the presence of LaCoO₃ as catalyst.

The hydrothermal synthesis of mixed metal oxides as anode materials in hybrid capacitors

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Poster Presentation P19

A materials discovery approach to nanoparticle synthesis was used to highlight lead compositions of mixed molybdenum, vanadium and niobium oxide nanoparticles for use in hybrid capacitor. Continuous Hydrothermal Flow Synthesis (CHFS) was used to produce high surface area mixed-metal oxide materials, which were subsequently electrochemically tested over a range of increasing current densities (C rates). The best performing material was found to exhibit specific capacities of 652 and 120 mAh g⁻¹ at 0.5 and 10 A g⁻¹ respectively. Analysis of Cyclic voltammetry testing of this lead material was used to determine that the pseudocapacitive contribution to the total charge storage was >80% suggesting that this material would perform well in a hybrid capacitor device.

Synthesis and functionalization of silica coated SPIONs for biomedical applications

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Poster Presentation P20

In the last decades magnetic iron oxide nanoparticles have been extensively investigated for their various biomedical applications such as diagnostic imaging, biological sensing, drug and cell delivery and cell tracking [1]. In this contest, this work focuses on the synthesis of silica coated Super Paramagnetic Iron Oxide Nanoparticles (SPION@SiO₂) [2] decorated with Au nanoparticles (NPs) and functionalized with biological molecules and in order to serve as functional nanomaterials for targeting liver cancer in theranostic applications. The synthetic parameters have been thoroughly investigated in order to define their effects on the nanostructure morphology. In particular, the amount of SPION and reagents as TEOS (Tetraethyl orthosilicate) and IGEPAL (Octylphenoxy poly(ethyleneoxy)ethanol) forming the microemulsion used for the silica shell growth, play a critical role on the multiplicity of the core in the final SPION@SiO₂ nanostructures and on their dimension. Subsequently, the SPION@SiO₂ have been coupled with Au seeds and bioconjugated with selected carbohydrates, β-D-galactose and β-D-lactose. These molecules are suitable to target liver cancer cells, since they are contained as terminal residues in asialoglycoproteins and, thus are able to selectively bind the specific receptor *hepatocyte lectin* ASGP-R1, which is overexpressed on the human hepatocarcinoma cell surface [3]. A systematic investigation of the prepared functional nanostructures has been carried out by complementary morphological, spectroscopic and magnetic characterization. The properties of the bioconjugates indicate that the proposed nanomaterial hold a great promise for future diagnostic and theranostic applications.

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[3] Kikkeri R., Lepenies B., Adibekian A., Laurino P., Seeberger P. H., *J. Am. Chem. Soc.* 2009, 131 (6), 2110-2112

High throughput synthesis of photocatalytic thin films and nanomaterials

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Poster Presentation P21

Whilst the amount of fresh water on the planet has remained relatively constant over time, continued recycled through the atmosphere and back onto the earth, the human population has dramatically grown, increasing water demand. The dearth of clean water sources due to the rapid development of industrialisation and metropolitan areas has led to shortages, that are exacerbated by droughts. All this has made access to drinking water a major issue that needs to be solved by both developing and developed worlds.

The amount of fresh water available to the world population represents only 2.5 % of all water in the planet. It is worth mentioning that most of this fresh water is trapped in glaciers and snowfields, leaving only 0.007 % of the planet's fresh water available to be used by human beings. It has been estimated that around 4 billion people worldwide have little to no access to clean water resources. This world scenario is expected to get worse, due to the increase of industrialisation and farming, which will release micropollutants and contaminants into the natural water cycle. The wastewater problem could be addressed by using conventional water treatment methods, such as ozonation, membrane bioreactors, electrocatalytic treatment and chlorination. However, these methods are highly expensive and energy intensive, making them largely inaccessible in developing countries. Hence, highly efficient and low-cost water treatment technologies must be developed and optimised. In this work, we present the use of photocatalysis to remove persistent organic compounds and micro-organisms from water streams. This is a low-cost and sustainable method that can be easily used in developing countries. The application of photocatalysis for remediation purposes has been explored through the synthesis of nanoengineered photocatalysts based on non-metal doped TiO₂ materials, as well as alternative non-TiO₂ photocatalysts with potential extended activity in the visible range. High throughput methods, namely continuous hydrothermal flow synthesis (CHFs) and chemical vapour deposition (CVD) were used to synthesise, optimise and explore new photocatalytic systems for water cleaning applications.

Continuous flow synthesis of pure and doped ZnS nanoparticles via a green microfluidic approach

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Poster Presentation P22

In recent years, microfluidic reactors have become highly attractive environments for synthesizing quantum dots of exceptional quality [1]. Two of the major benefits of using microfluidic systems to synthesize nanomaterials are (i) the rapid and continuous mixing of liquid precursors, that ensures the formation of homogeneous reaction mixtures on a millisecond time scale, and (ii) the ability to dynamically change reaction conditions such as reagent concentrations and reaction time. Thanks to these, microfluidic techniques allow a precise control over the final product. The aim of this study is to synthetize pure and doped (with luminescent ions such as Mn²⁺, Cu²⁺, Ni²⁺, Eu³⁺, Sm³⁺, Nd³⁺, Yb³⁺) ZnS nanoparticles via a green (in water at room temperature) microfluidic approach, with fine control over the product size. The crystalline structure, size and morphology of the synthesized products were analysed employing X-Ray Diffraction (XRD) and TEM analysis, while the surface composition was determined by X-Ray Photoelectron Spectroscopy (XPS). The luminescence properties of the synthetized doped ZnS nanoparticles were also studied in view of a possible application in the optical bioimaging field.

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Synthesis of alloy NPs by laser ablation and investigation of their properties for biomedical imaging

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Poster Presentation P23

In recent years, the technique of laser ablation in liquid environment (LASiS) has created a lot of interest due to its low cost, versatility and easy of execution. Among its main advantages, there is also the fact that laser ablation satisfies the 12 principles of “green chemistry”.

In this study, LASiS was used to synthesize nanoparticle alloys to be employed as biocompatible multimodal contrast agents (MCAs) in biomedical imaging, such as MRI and CT, and for a special type of therapy, the boron neutron capture therapy (BNCT).

The two alloys on which we focalized our attention are iron-gold and iron-boron. The choice of these materials was dictated by their chemical and physical properties: 1) all the three metals are biocompatible, a key point for biomedical applications; 2) iron has excellent magnetic properties, for this reason it's a very good contrast agent; 3) gold is easily functionalizable with biocompatible polymers; 4) finally, boron was chosen because it can accumulate in tumoral cells and, thanks to its good interaction with thermal neutrons, can make the nanoparticles relevant for BNCT.

The synthesized NPs were characterized with various techniques: TEM was used to study their size distribution and their morphology; XRD was performed to determine the crystallographic structure of the materials and finally ICP and XPS were used to describe the ratio and the oxidation state of the elements in the alloys, respectively. According to the preliminary tests, these NPs showed promising results for theranostic applications.

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Synergic deposition route for the functionalisation of biomedical devices

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Poster Presentation P24

Titanium has been widely used for dental implants due to its biocompatibility, corrosion resistance, and mechanical properties. In order to improve osseointegration, the Ti surface is generally functionalized. A typical methodology for surface modification is the coating of Ti substrates with bioactive layers of calcium phosphate ceramics (CPCs) [1]. However, CPC coatings on metal implants usually suffer from poor adhesion. With the aim of improving the adhesion strength, the insertion of dense and compact ceramic interlayers is reported to be useful^[1]. Among various ceramics, crystalline TiO₂ has been extensively used thanks to its well-known biocompatibility and bioactivity [2].

In this work, a multi-step solvent free process is proposed, with the aim of obtaining a final composite material made up of a dense, compact and crystalline titania inter-layer (obtained via Metal Organic Chemical Vapour Deposition technique) and of a homogeneously spread discontinuous CPC top-layer, with particular chemical composition, crystallinity and morphology (obtained by means of water-based spray pyrolysis technique). Finally, a thermal treatment is carried out. These synthesis approaches are relatively simple and economic, eco-compatible and consequently suitable for an easy industrial scale-up of the process.

The morphology, crystalline structures and wettability of the coated surfaces is here presented. Moreover, ions release and in vitro acellular bioactivity have also been evaluated.

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Halloysite nanotubes as support for nanocatalysts

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Poster Presentation P25

Halloysite nanotubes (HNTs) are aluminosilicates with a chemical composition similar to kaolinite, $\text{Al}_2(\text{OH})_4\text{Si}_2\text{O}_5 \cdot n\text{H}_2\text{O}$, consisting of two connected layers rolled up into hollow tubular structures. Their length distribution varies from 200 nm to 2 μm , the internal diameter between 15 and 25 nm and the external one from 30 to 100 nm. In this naturally occurring form, the silica part is externally exposed, while the alumina layer faces at the lumen wall. In this work, we have explored the possibility to use HNTs as support for different metals, to be used as heterogeneous catalysts [1]. To this aim, the HNTs external surface has been treated with a piranha solution, in order to increase the number of available silanol groups. Then, the activated surface has been functionalized with aminopropyl triethoxysilane, to provide reactive amino groups. The last ones have been used for a post-functionalization step to grow nanoparticles (NPs) of Au, Ag and Ru upon reduction with NaBH_4 of their corresponding metal salts [2].

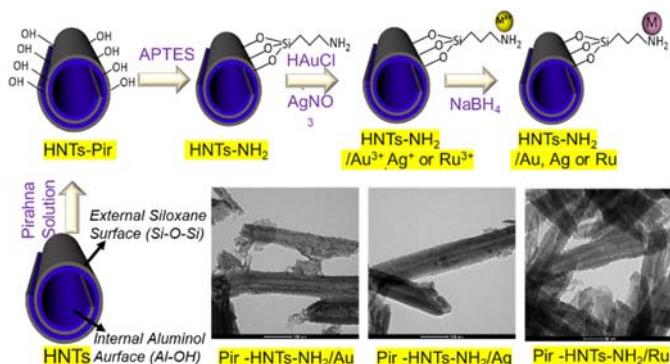


Figure 1: Synthesis of the metal NPs immobilized on HNTs and their TEM images.

In particular, the functionalized HNTs with Au NPs (2~10 nm) perform, with good activity and selectivity, the oxidation of furfural to yield furoic acid under an oxygen atmosphere, with 95% conversion in 6 h at 80°C. Moreover, the functionalized HNTs can be used as efficient catalyst for the reduction of 4-nitrophenol to 4-aminophenol, using NaBH_4 as reductant, with 100% conversion and selectivity for 4-aminophenol in 120 s. The above results demonstrate the possibility to use HNTs as supports for catalytic units.

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Wet-chemistry synthesis of metal sulphides nanoparticles at very low temperature

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Poster Presentation P26

Transition metal sulphides are a manifold class of binary compounds, interesting for their functional properties and with wide fields of implementation [1]. Six metal sulphides -ZnS, CuS, PbS, NiS, MnS, SnS- have been prepared through a green, easy and reproducible synthesis route, based on the precipitation of the compounds in aqueous solutions. The sulphides were prepared starting from earth abundant metal salts and Na₂S, dropping the metal solution very slowly in order to favour nucleation over growth. Despite the common use of high temperature, the aim of the study has been to obtain crystalline nanoparticles working at 0°C. The sulphides have been analysed employing X-Ray Diffraction (XRD), X-Ray Photoelectron Spectroscopy (XPS) and Transmission Electron Microscopy (TEM). Nanostructures with diameter range between 3 and 20 nm have been observed by TEM. Thanks to XPS, a good level of purity has been confirmed, while XRD has shown different degrees of crystallinity for each of the six different sulphides, pointing out a spurious hydroxide phases in the case of MnS and NiS. This study has disclosed exciting perspectives in the green and low temperature synthesis of functional sulphides nanostructures with controlled crystallinity and size.

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Preparation of mesoporous $\text{SrTi}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ solid solutions with tunable porosity

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Poster Presentation P27

Perovskite oxides can be considered as a very versatile class of materials suitable for a wide range of applications, from heterogeneous catalysis, to electronics thanks to the ease in accommodating high amount of oxygen vacancies without compromising their structural stability. However, the poor textural properties still limit the oxygen mobility and the potential catalytic applications [1]. The wet-synthesis of perovskite oxide materials is usually based on molar excess of chelating agents, such as citric acid and ethylene glycol, used to ensure homogeneous mixing of the cations at the molecular scale and avoid secondary phase formation [2]. Using a modified version of this approach, i.e. by substituting the standardly used ethylene glycol with longer chain polyols, we successfully synthesized mesoporous $\text{SrTi}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ (STF) with tunable (as a function of polyol length) specific surface area up to $80 \text{ m}^2/\text{g}$ and homogeneous dispersion of the ions within the perovskite lattice. Microstructure, morphology and composition of the oxide materials were investigated by means of XRD, SEM/EDX and N_2 physisorption. To estimate the effect of the improved textural properties, the solid solutions were tested as catalysts for methane oxidation.

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Degenerately doped zinc oxide nanocrystals as plasmonic gas sensors.

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Poster Presentation P28

Gas sensing has a great influence in many areas across a wide range of applications, including ensure safety via detection of dangerous or flammable gases in different environments, monitor feedstocks and air pollutants, public security and automotive applications [1]. An optical sensing approach instead of more common electrochemical sensing approach offers faster response, flexibility, higher thermal resistance, absence of electric contacts and electric current, and it is cheaper, not easily poisoned, not affected by electrical and magnetic fields [2].

In this work we have used ZnO doped with trivalent cations (Al^{3+} and Ga^{3+}) or tetravalent cations (Si^{4+} and Ge^{4+}) with doping concentration of 20 % as plasmonic gas sensor, using an innovative non-aqueous heat up colloidal synthesis [3]. It is proved by spectrophotometric analysis that introduction of doping agent causes the formation of a surface plasmon resonance in the near infrared, tunable changing concentration and dopant nature. Strong sensitivity of the plasmon resonance to chemical variations at the surface of the nanocrystal make this category of materials very suitable for detection of reducing and oxidizing gases. NO_2 sensing is presented due to the strategical importance of this gas for human health increased likelihood of respiratory problems such as wheezing, coughing, colds, flu, bronchitis and its emission derive from fossil fuel combustion and incineration.

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Hydrothermal synthesis of Bi₂Se₃ platelets

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Poster Presentation P29

Bismuth selenide (Bi₂Se₃) is one of the most investigated topological insulators (TIs). Due to its topological surface states (TSS) it displays special electronic and optical properties, which makes Bi₂Se₃ a good candidate for a variety of important applications, e.g. photodetectors, ultrafast lasers, cancer treatment, thermo-electronics, spintronics etc. [1].

Bi₂Se₃ displays a quasi-layered crystal structure, which makes it suitable to grow into different two-dimensional structures suitable for a variety of applications and devices [2]. To realize the new devices and exploit the unique Bi₂Se₃ properties, it must be directly contacted with another semiconductor or a metal [3].

According to the literature, the BIS nanoplatelets, could only be synthesized using a solvothermal method [2, 4, 5]. The drawback of this method is use of toxic and expensive organic solvents. Moreover, after the solvothermal synthesis, the particles are coated with a thin amorphous layer that is formed by adsorption of the organic molecules. The formed organic layer is detrimental for the device application of Bi₂Se₃ because it impedes the direct contact between Bi₂Se₃ and the other materials in the heterostructure.

Because of the drawbacks of solvothermal method, we investigate the possibility to synthesize the Bi₂Se₃ nanoplatelets with simple hydrothermal method. For the synthesis of the Bi₂Se₃ nanoplatelets, bismuth and selenium reactants were dissolved in distilled water. The ions are then precipitated with addition of aqueous NaOH. At the end, hydrazine was added as a reductive agent. The homogeneous suspension was sealed in an autoclave and treated at different temperatures for different time. After the synthesis the particles were washed, dried and characterized using XRD, SEM and HRTEM. With hydrothermal method we successfully synthesized Bi₂Se₃ nanoplates. HRTEM analysis revealed that Bi₂Se₃ synthesized by hydrothermal method had no amorphous layer adsorbed onto their surface. Therefore, such particles have potential to be used as building block for heterostructures.

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Amendola	Vincenzo	P23 (97)
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Bauer	Dustin	OP4 (40), FP1 (63), P3 (77)
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