DAYS

Chemistry for Innovative Materials

Martedì 27 Maggio 2014, ore 14.15, aula 12 Via Quarello 15

14:15-14:30 Functional and Structural Metallic Materials
Livio Battezzati (10 min di discussione)

14:40-14:55 Nanocomposites: Industrial opportunity or challenge
Marco Zanetti

14:55-15:10 Graphene-like materials based nanocomposites for optical and electrical applications.
Domenica Scarano

15:10-15:30
Discussione

15:30-15:40 Commissione Spokes

15:40-16:00 Coffee Break (networking)

16:00-16:15 Molecularly imprinted materials from sacrificial porous silica: synthesis, binding properties and perspectives
Cristina Giovannoli

16:15-16:30 Utilizzo di sostanze bio-organiche estratte da rifiuti per la produzione di materiali di interesse ambientale
Giuliana Magnacca

16:30-16:50
Discussione

16:50-17:05 Laboratory characterization of MOFs: a fundamental step towards industrial applications
Francesco Bonino

17:05-17:20 Beyond adsorption properties of MOF: a computational study
Bartolomeo Civalleri

17:20-17:40
Discussione

17:40-17:55 High Tc Superconductors. Synthesis (HTSC), characterization, modeling and applications
Angelo Agostino (10 min di discussione)

18.05 chiusura

Functional and Structural Metallic Materials

L.Battezzati, M.Baricco, P.Rizzi, A.Castellero, G.L.Fiore, Postdocs and PhD students

Most of the metals in the Periodic Table are used as solids to make materials for components either because of their functional properties (chemical, magnetic, electrical,...) or of their mechanical strength. We propose a description of current activities on a few topics showing their scientific and technological motivation and outlining the applications of materials:

- bulk and porous precious metals: electro-catalysis, SERS, corrosion and aesthetics ...,
- accelerating the discovery of new alloys and processes: high entropy alloys, magnets,
- material characterization: structural, thermal. mechanical, electrochemical.

Aspects to be detailed for interaction in the Department include: fine and local chemical analysis, some electrochemical and spectroscopic techniques, mechanical characterization.

Nanocomposites: Industrial opportunity or challenge?

Marco Zanetti

Polymer nanocomposites represent a new class of multiphase materials containing dispersion of nano-sized filler materials such as nanoparticles, nanoclays, nanotubes, nanofibers etc. within the polymer matrices. Owing to their nanoscale size features and very high surface-to-volume ratios, they possess unique combination of multifunctional properties not shared by their more conventional composite counterparts reinforced with micro-sized fillers.

Despite the proven benefits of nanocomposites such as mechanical properties, barrier properties and contribution to fire retardancy, polymer nanocomposites are used today only in niche applications. The reasons for the limited growth of nanocomposites are explained through dispersion challenges and inferior oxidative and photooxidative stability. The talk will be focused on the relationship between structure and properties and to the interdisciplinary approach required for the nano-morphology characterization.

Graphene-like materials based nanocomposites for optical and electrical applications

Domenica Scarano, Federico Cesano

Graphene like materials including carbon nanotubes (CNTs), titanates nanotubes (TNTs), few-layers graphite nanoplatets (GNPs) or nanosized MoS_2 have experienced a rapid growth, due to their unique optical, photocatalytic and electrical properties correlated with the 1D (CNTs, TNTs) or 2D ultrathin atomic layer structure (Graphene, MoS_2). However, to exploit their full potential, it is often necessary to combine them even with other materials to achieve optimal filler exfoliation/dispersion or to overcome restacking phenomena. Carbon-based nanofillers such as Expanded Graphite (EG), Graphite Nanoplateles (GNPs) or Carbon Nanotubes (CNTs) have been combined with polymers to generate enhancements in localized conductivity, to be used in sensing devices or in electric circuits. Remarkable advantages come also from the combination of different type of fillers (i.e. 1D, 2D and 3D), which, for example, can help in reducing the electric percolation threshold. To this aim, the role of the synergistic effect between 1D CNTs and 2D GNPs fillers on the electrical properties of GNPs/CNTs/polymer composites has been highlighted. The composites were characterized by electrical measurements, XRD analysis, SEM (conventional and at low potentials), optical microscopies, to correlate conductivity with particle morphology and filler dispersion

Besides, MoS_2/titanates nanocomposites are of great interest for photocatalytic applications. Titanates combine the properties of TiO_2nanoparticles (e.g., wide band gap semiconductor photocatalyst) with the properties of layered systems (e.g. high surface area for improved interfacial contact). As MoS_2 has the same layered structure of graphene with similar properties and absorbs in the visible range, we focused on hybrid materials, made by TNTs sensitized with exfoliated MoS_2 , in order to increase the adsorption ability of titanate and to obtain a new material with high photocatalytic performance. Following this line, in this work exfoliated MoS_2/ porous titanate

nanocomposites have been synthesized and characterized by AFM, TEM, Raman and UV-Vis-NIR spectroscopies, to correlate optical properties with morphology and structure.

Molecularly imprinted materials from sacrificial porous silica: synthesis, binding properties and perspectives

Cristina Giovannoli

The most popular method for obtaining molecularly imprinted polymers consists in a bulk polymerisation which produces a monolithic material that has to be crushed and sieved to obtain particles of the desired size distribution. Despite being a convenient approach, it shows many practical drawbacks.

With the purpose of overcoming these drawbacks, one of the most recent methodologies consists in filling the pores of meso- or macroporous silica beads with an imprinting mixture, polymerizing it and dissolving the inorganic support, leaving porous imprinted beads as a negative image of the sacrificial silica beads. Templates can be introduced within the silica beads together with the pre-polymerization mixture or previously covalently grafted to the inner surface of the pores.

The use of sacrificial silica beads as microvessels for the synthesis of molecularly imprinted beads is particularly convenient when a fragmental or mimic template approach is needed or when compatibility between template molecule and porogenic solvent does not exist.

Bio-organic substances extracted from wastes for the production of materials for environmental applications

Giuliana Magnacca, Debora Fabbri, Enzo Laurenti, Alessandra Bianco Prevot, Postdocs, PhD students

Green wastes after composting are sources of substances of various molecular weight containing aliphatic chains substituted by aromatic rings and functional groups such as COOH, CON, CO, PhOH and others. These substances show surfactant properties and can be used as binders and/or templating agents for the production of monoliths and/or mesoporous powders, or can be immobilized as active phases for adsorption and/or photodegradation of pollutants in aqueous solution. Aim of this research is to reduce the environmental impact of petroleum-based reactants using non-petroleum-based intermediates and to valorise the differential collection of wastes through the production of materials for environmental applications ("waste cleaning waste").

Laboratory characterization of MOFs: a fundamental step towards industrial applications

Francesca Bonino, Carlo Lamberti, Silvia Bordiga, PhDs students and Postdocs

Crystalline nanoporous metal–organic frameworks (MOFs), constructed from metal ions and organic linkers, offer vast potential for the design of porous materials with molecularly selective interfaces, novel physical properties, enormous surface areas and a diverse array of functionality. After the first reports on metal organic frameworks, the main focus in the field was the discovery of unknown structures. More recently, the attention has moved towards utilizing the materials, and applications within the fields of catalysis, gas storage, separation and drug delivery have been reported. For the aim of further applications, also fundamental knowledge, as insight in formation and stability, is of great importance.

In case of complex structures such as MOFs, the supramolecular architecture given by the tridimensional organization of the organic linkers and metal ions forming specific secondary building units (SBU), require advanced characterization techniques. Many spectroscopic methods, ranging from IR, Raman, XAFS, RIXS, UV-Vis-NIR to Luminescence have been employed.

An understanding of the structural, physical and chemical properties of the materials have been pursued considering the properties of samples as prepared, their changes upon activation, their reactivity towards probe molecules, adsorbents and reagents. This characterization step is considered fundamental towards the field of industrial applications.

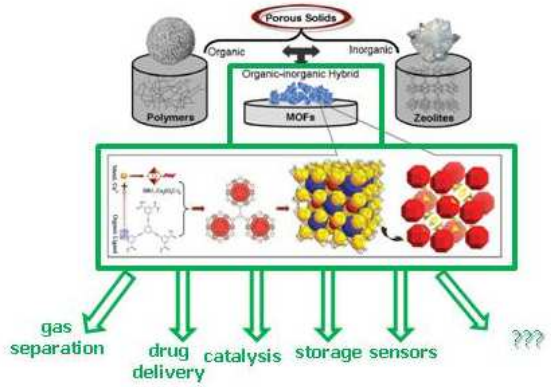

Figure 1. Possible applications of MOF materials

Beyond adsorption properties of MOF: a computational study
Bartolomeo Civalleri
I metal organic framework sono considerati dei materiali innovativi e con grandi potenzialità per lo sviluppo tecnologico. Ne è dimostrazione il numero sempre crescente di strutture sintetizzate e di pubblicazioni relative al loro studio. Inoltre, è in crescita l'interesse da parte delle industrie per applicazioni in diversi settori: dalla cattura, purificazione e stoccaggio di gas alla catalisi, dalla sensoristica, optoelettronica al rilascio controllato di farmaci.
Il successo dei MOF risiede nella loro struttura reticolare basata sulla combinazione di un cluster inorganico multi-metallico, che funge da nodo, e un legante organico che agisce come uno spaziatore. Il risultato è una struttura cristallina solitamente porosa. Questo rende i MOF dei materiali molto versatili per l'ampia possibilità di modificare il cluster e il legante, modulandone le proprietà chimico-fisiche.
Negli ultimi anni c'è stata nel nostro dipartimento un'intensa attività di modellizzazione di MOF principalmente legata alla loro capacità di adsorbimento, ma anche altre proprietà sono state studiate e potrebbero essere sfruttate. In questo contributo, verranno quindi discusse proprietà dielettriche, elastiche e magnetiche di MOF ottenute da calcoli ab initio e si cercherà di fornire degli spunti per possibili applicazioni alternative dei MOF (es. sensoristica, elettronica, …).

High Tc Superconductors. Synthesis (HTSC), characterization, modeling and applications.
Angelo Agostino
The research, developed in the past years, has been devoted to the synthesis, characterization and development of high critical temperature superconductors. In particular, the structural changes induced by the use of suitable substituents helpful to the morphological micrometric control and to the increasing of the purity degree of these materials has been investigated. The micro crystals HTSC, characterized by a multi-layered structures and by a high spatial order, are the best candidates for the realization of THz devices based on Intrinsic Josephson junctions (IJJ). The realization of these devices is the dissemination phase of the developed research.