DAYS #9
Chemistry for Environment

Mercoledì 09 Luglio 2014, ore 9:00, aula D1

Introduzione: C. Minero e F. Turci

9:00-9:15 - **Photochemical processes in surface waters**
Davide Vione, Marco Minella, Elisa De Laurentiis, Valter Maurino, Claudio Minero
(10 min di discussione)

9:25-9:40 - **NH_3-SCR of NO_x over Cu-zeolites for Diesel engine applications**
Filippo Giornadino, Elisa Borfecchia, Kirill Lomachenko, Silvia Bordiga and Carlo Lamberti
(10 min di discussione)

9:50-10:05 **Asbestos in the environment: a multidisciplinary approach to deal with the potential health hazard**
Ingrid Corazzari, Ivana Fenoglio, Bice Fubini, Arianna Marucco, Cristina Pavan, Maura Tomatis, Francesco Turci
(10 min di discussione)

10:15-10:30 **TiO_2-based process as a tool to assess the fate of emerging contaminants in aquatic systems**
Debora Fabbri, Paola Calza, Claudio Minero
(10 min di discussione)

10:40-10:50 - **Commissione Spoke**

10:50-11.15 - **Coffee break (discussion)**

11:15-11:30 **Development and applications of voltammetric sensors for the determination of metal ions and pharmaceutical compounds**
Agnese Giacomino, Ornella Abollino
(10 min di discussione)

11:40-11:55 **Functionalized silicas for environmental and analytical applications**
M.C. Bruzzoniti, C. Sarzanini, R.M. De Carlo, L. Rivoira
(10 min di discussione)

12:05-12:20 **Intelligent polymers for environmental contaminants**
C. Baggiani
(10 min di discussione)

12:30-12:45 **Studies on pollution trends in anthropized and polar areas**
Mery Malandrino
(10 min di discussione)

12.55 **Termine dei lavori**

Photochemical processes in surface waters

Davide Vione, Marco Minella, Elisa De Laurentiis, Valter Maurino, Claudio Minero

The photochemical reactions taking place in natural waters play a key role in the degradation of organic pollutants and of natural organic molecules, thereby also influencing the carbon cycle in inland water bodies. The cited processes are usually divided into direct photolysis and indirect photochemistry, the latter involving photoinduced transient species such as $^{\bullet}OH$, $CO_3^{-\bullet}$, $^1O_2$ and ^{3}CDOM* (triplet states of chromophoric dissolved organic matter), produced by irradiation of photosensitisers such as CDOM, nitrate and nitrite. Recent research by our group in this field has led to the successful modelling of surface-water photochemistry (modelling results have been validated against field data) and to the development of a dedicated software (APEX: Aqueous Photochemistry of Environmentally-occurring Xenobiotics). The software availability enables the prediction of the photochemical fate of pollutants and it is a key tool to link photochemical processes in inland waters with climate change.

NH_3-SCR of NO_x over Cu-zeolites for Diesel engine applications

Filippo Giornadino, Elisa Borfecchia, Kirill Lomachenko, Silvia Bordiga and Carlo Lamberti

For the last 15 years or so, the catalysis community has been addressing the challenge of reducing NOx under the highly oxidazing (learn burn) conditions encountered in the exhaust of Diesel-powered vehicles. Selective catalytic reduction of NOx with ammonia (NH3-SCR) is an effective way to remove hazardous NOx gas compounds from the exhaust of lean-burn engines. Among the various catalysts tested for this purpose, significant research efforts focus on small pore Cu-exchanged zeolites due to their improved hydrothermal stability and activity over a wide range of temperature if compared with medium pore zeolites, e.g. Cu-ZSM-5. Conversion mechanism over Cu-zeolites is still under debate and a complete picture of the structure-activity relationship for Cu-zeolites in NH3-SCR applications is still missing. Since the reaction mechanism involves the redox cycle of Cu+/Cu2+ and the change of local geometry of copper due to interaction with strong ligands, e.g. NH3, the combination of different spectroscopic techniques is at the basis of clarifying the chemistry of the catalytic process. This work, is performed within a collaboration with Haldor Topsøe A/S.

U. Deka, I. Lezcano-Gonzalez, B. M. Weckhuysen and A. M. Beale, ACS Catal., 2013, **3**, 413.
S. Brandenberger, O. Krocher, A. Tissler and R. Althoff, Catal. Rev., 2008, **50**, 492.
F. Gao, J. Kwak, J. Szanyi and C. F. Peden, Top. Catal., 2013, 56, 1441.
D. W. Fickel, E. D'Addio, J. A. Lauterbach and R. F. Lobo, Appl. Catal. B-Environ., 2011, **102**, 441.
F. Giordanino, P. N. R. Vennestrom, L. F. Lundegaard, F. N. Stappen, S. L. Mossin, P. Beato, S. Bordiga and C. Lamberti, Dalton Trans., 2013, **42**, 12741.
F. Giordanino, E. Borfecchia, K. A. Lomachenko, A. Lazzarini, G. Agostini, E. Gallo A. V. Soldatov, P. Beato, S. Bordiga and C. Lamberti, Interaction of NH_3 with Cu-SSZ-13 Catalyst: A Complementary FTIR, XANES, and XES Study. J. Phys. Chem. Lett. 2014, **5**, 1552

Asbestos in the environment: a multidisciplinary approach to deal with the potential health hazard

Ingrid Corazzari, Ivana Fenoglio, Bice Fubini, Arianna Marucco, Cristina Pavan, Maura Tomatis, Francesco Turci

Naturally occurring asbestos (NOA) are widely diffuse in several countries. In Italy, asbestos bearing rocks are mainly located in North-western Alps.

An overview of the researches carried out by the TBM group will be presented, focusing the attention on the multidisciplinary approach employed to evaluate the potential health hazard for people living in NOA surrounding.

The evaluation of the potential toxicity of fibrous minerals, the measurement of airborne fiber dispersion in the environment, and the development of new detoxification strategies for waterborne asbestos fibers will be presented.

TiO_2-based process as a tool to assess the fate of emerging contaminants in aquatic systems

Debora Fabbri, Paola Calza, Claudio Minero

We point on the fate of emerging contaminants in surface waters, groundwater and drinking water, with emphasis on pharmaceuticals, focusing on their degradation and on the identification of their transformation products. The study of their degradation processes becomes important in understanding their toxic effects in the aquatic environment and, in particular, on human beings. As the standards for field evaluation of biological metabolites, and products of hydrolysis, redox and photochemical reactions are not available, we demonstrated that TiO2-based degradation products in many cases produces compounds that can be found in the environment. Initially, laboratory experiments were performed to artificially produce degradation compounds similar to those formed in oxidation/reductive pathways by adopting a photocatalytic process as a model-system and, afterwards, to identify them in real samples, beside parent compounds. This approach was successfully used and permitted to identify several TPs, alongside the parent compounds, in water samples. Acute toxicity related to these EPs and to their transformation products was evaluated, too.

Development and applications of voltammetric sensors for the determination of metal ions and pharmaceutical compounds

Agnese Giacomino, Ornella Abollino

The determination of metals and residuals of pharmaceuticals at trace levels is an important issue in the environmental field. Metal ions are usually determined by atomic spectroscopy or by ICP mass spectrometry, whereas chromatography, coupled to mass spectrometry, is adopted for the determination of pharmaceuticals. Electroanalytical techniques represent attractive alternatives to these approaches, since they are sensitive, relatively inexpensive and offer speciation capabilities. Our research group has developed a gold nanoparticle-modified glassy carbon sensor (AuNPs-GCS) and, after optimization of the experimental conditions, has applied it to the determination of mercury in environmental matrices (water, sediments, particulate matter, plants), food and drugs. The status of the gold surface has been examined. We are presently studying sensors based on carbon paste and

ionic liquids, functionalized with AuNPs, both for mercury and trace pharmaceuticals determination. The main findings and critical issues in this research field will be addressed.

Functionalized silicas for environmental and analytical applications

M.C. Bruzzoniti, C. Sarzanini, R.M. De Carlo, L. Rivoira

Mesoporous silica-based materials show extremely interesting adsorption properties towards target species when provided with organic functions that modify the physico-chemical properties of the surface. These properties are enhanced from the very high internal surface and the acceptable stability in a quite wide range of pH typical of these materials. The study of the interactions substrate-analytes is of paramount importance in order to enhance the retention performance of the substrates.

In the last years, research by our group has been focused on the synthesis and characterization of silica-based materials properly functionalized for the removal of species of environmental relevance, such as transition metal ions and disinfection by-products of water potabilization processes. The main results achieved will be discussed throughout this presentation.

Intelligent polymers for environmental contaminants

C. Baggiani

This line of research was born from the experimental demonstration of the existence of a relationship between the recognition properties of molecularly imprinted polymers and their corresponding not-imprinted polymers. As a consequence, by direct screening of polymeric libraries characterized by molecular diversity, it is possible to identify not-imprinted polymers with binding properties for given analytical targets and use them to efficiently clean-up environmental matrices

Studies on pollution trends in anthropized and polar areas

Mery Malandrino

Atmospheric pollution resulting from airborne particulate matter continues to be a major problem since epidemiological studies have established a linkage between the amount of the PM_{10} and its elemental concentration with adverse respiratory health effects and, at a larger scale, the ongoing climate changes.

In particular, Arctic regions are showing to be the first areas affected by the present climatic variations. Consequently, the study of the chemical composition of atmospheric aerosol in the polar areas is important to understand the feedback processes between the climate forcing and the environmental responses.

Moreover, to understand the current status of atmosphere, both in remote and anthropized areas, it is necessary to know the temporal trends of element composition present in airborne particulate matter sampled at different monitoring stations for long periods of time.