

**ADHOC 2008 PROGRAM**

**San Servolo Island, Venice (Italy)**

**20 – 25 July, 2008**

## Sunday July 20<sup>th</sup>

15:00 – 18:30 Registration

18:30 – 20:00 Get Together

## Monday July 21<sup>st</sup>

9:00 – 9:30 Opening

Chairperson: Luigi Casella

9:30 – 10:20 **PL1:** John T. Groves (Princeton University, USA): - How Nature Uses Oxygen - Lessons from Enzymes and Model Compounds

10:20 – 10:50 **IL1:** WonWoo Nam (Ewha Womans University, Korea): Mononuclear Non-Heme Iron(IV)-Oxo Complexes in Oxygenation Reactions

10:50 – 11:20 Coffee Break

Chairperson: Tsutomu Katsuki

11:20 – 11:40 **O1:** Miguel Costas (Universitat de Girona, Spain): Bioinspired alkane and alkene oxidations with nonheme iron complexes that challenge the oxygenase paradigm

11:40 – 12:00 **O2:** Yoshinori Naruta (Kyushu University, Japan): Selective preparation of end-on ferric-peroxo, ferrous-superoxo, and ferric-hydroperoxo species in solution

12:00 – 12:20 **O3:** Ariane Brausam (University of Erlangen Nürnberg, Germany): Detection of Reactive Intermediates in Oxidation Reactions Catalyzed by Fe(III)-Porphyrins

12:20 – 12:40 **O4:** Alexander B. Sorokin (IRCELYON, France): Bio-inspired chemical system oxidizes methane under physiological conditions

12:40 – 13:10 **IL2:** Marco d'Ischia (University of Naples, Italy): The moving frontiers of melanin research: chasing transient (semi)quinones in 5,6-dihydroxyindole polymerization

13:10 – 15:00 Lunch

Chairperson: John T. Groves

- 15:00 – 15:50 **PL2:** Vincent L. Pecoraro (University of Michigan, USA): Computationally Assisted Design of Asymmetric Sulfoxidation Catalysts based on Functional Models for Vanadium Dependent Haloperoxidases
- 15:50 – 16:10 **O5:** Sabine Laschat (Universität Stuttgart, Germany): Novel non-heme iron complexes: synthesis, spectroscopic characterization and catalytic properties in allylic and aerobic C-H oxidations
- 16:10 – 16:30 **O6:** Brian R. James (University of British Columbia, Canada): O<sub>2</sub>-oxidation of thiols catalyzed by Ru-porphyrin complexes
- 16:30 – 17:00 Coffee Break

Chairperson: Jim Mayer

- 17:00 – 17:50 **PL3:** Jim Barber (Imperial College London, UK): Photosystem II where dioxygen is generated
- 17:50 – 18:10 **O7:** Matthew W. Kanan (Massachusetts Institute of Technology, USA): Efficient oxidation of neutral water to dioxygen with a catalyst composed of earth-abundant materials
- 18:10 – 18:30 **O8:** Stefan Bernhard (Princeton University, USA): Efficient and Tunable Catalysts for the Oxidation of Water

## Tuesday July 22<sup>nd</sup>

Chairperson: Armin Liebens

- 9:00 – 9:40 **KL1:** Alain Vandebussche (Solvay S.A., Belgium): Hydrogen peroxide - A view from industrial perspective
- 9:40 – 10:10 **IL3:** Raffaele Saladino (University of Tuscia, Italy): Production of maleic anhydride from cellulose wastes by activation of hydrogen peroxide with rhenium homogeneous and heterogeneous
- 10:10 – 10:40 **IL4:** Giorgio Strukul (Università di Venezia, Italy): Soft Lewis Acids and Hydrogen Peroxide: a Viable Catalytic Approach to the Epoxidation of Simple Alkenes
- 10:40 – 11:10 Coffee Break

Chairperson: Shannon S. Stahl

- 11:10 – 11:40 **IL5:** Ronald Hage (Rahu Catalytics, The Netherlands): Applications of Mn-triazacyclononane bleaching catalysts
- 11:40 – 12:10 **IL6:** T. Daniel P. Stack (Stanford University, USA): Heterogenization of oxidation catalysts on high-surface area materials
- 12:10 – 13:00 **PL4:** Henrique Teles (BASF SE, Germany): Oxidation from an industrial perspective
- 13:00 – 15:00 Lunch

Chairperson: Oxana A. Kholdeeva

- 15:00 – 15:30 Flash presentations
- 15:30 – 16:30 Poster Session

Chairperson: Gianfranco Scorrano

- 16:30 – 17:00 **IL7:** Michele Rossi (Università degli Studi di Milano, Italy): Aerobic oxidation by gold nanoparticles: molecular aspects and applications
- 17:00 – 17:20 **O9:** Valerie Caps (IRCELYON, France): Understanding oxygen activation in the gold-catalyzed aerobic epoxidation of stilbene

- 17:20 – 17:40 **O10:** Christian Limberg (Humboldt-Universität zu Berlin, Germany): Oxidative dehydrogenations with O<sub>2</sub>: insights from novel homogeneous oxovanadium catalysts inspired by V<sub>2</sub>O<sub>5</sub>/SiO<sub>2</sub> surface species
- 17:40 – 18:00 **O11:** Matteo Guidotti (CNR – Istituto di Scienze e Tecnologie Molecolari, Italy): High oxidant efficiency with H<sub>2</sub>O<sub>2</sub> over grafted Ti-SiO<sub>2</sub> catalysts. The liquid-phase selective epoxidation of cyclohexene
- 18:00 – 18:50 **PL5:** Markus Antonietti (Max Planck Institute, Germany): Metal free catalysis with carbon nitride semiconductors, as well as some metal support

## Wednesday July 23<sup>rd</sup>

Chairperson: Markus Antonietti

- 9:00 – 9:50 **PL6:** Craig L. Hill (Emory University, USA): Terminal noble-metal oxo groups and stable molecular catalysts for H<sub>2</sub>O oxidation
- 9:50 – 10:20 **IL8:** Oxana A. Kholdeeva (Boreskov Institute of Catalysis, Russia): Ti-Catalyzed Selective Oxidations: From Single-Site to Double-Site Catalysts
- 10:20 – 10:40 **O12:** Delina Barats (Weizmann Institute of Science, Israel): A stable "end-on" iron(III)-peroxo complex in water derived from a multi iron(II) substituted polyoxometalate and molecular oxygen
- 10:40 – 11:10 Coffee Break

Chairperson: Michele Rossi

- 11:10 – 11:40 **IL9:** Ira A. Weinstock (Ben Gurion University, Israel): Outer-sphere oxidation of the superoxide radical anion
- 11:40 – 12:00 **O13:** Alessandra Molinari (Università degli Studi di Ferrara, Italy): Oxidative photocatalysis with W<sub>10</sub>O<sub>32</sub><sup>4-</sup> by O<sub>2</sub>: from homogeneous to heterogeneous systems
- 12:00 – 12:20 **O14:** Veronique Nardello-Rataj (Université de Lille I, France): Catalytic oxidation in three-liquid-phase microemulsion systems versus phase-transfer catalysis in two-liquid phase systems
- 12:20 – 12:40 **O15:** Isabel Santos Vieira (University of Aveiro, Portugal): A catalytically active peroxotungstate for the oxidation of alkanes and alkenes with H<sub>2</sub>O<sub>2</sub>
- 12:40 – 13:10 **IL10:** Paul L. Alsters (DSM, The Netherlands): Upscaling of "dark" singlet oxygenation
- 13:10 – 15:00 Lunch
- 15:00 – 16:00 Poster Session

## Thursday July 24<sup>th</sup>

Chairperson: Paolo Scrimin

- 9:00 – 9:50 **PL7:** Albrecht Berkessel (Universität zu Köln, Germany): Oxidation Catalysis by Hydrogen Bonding
- 9:50 – 10:10 **O16:** Olga Bortolini (Università della Calabria, Italy): Eco-friendly, organocatalytic epoxidations with oxone and sodium perborate in aqueous conditions
- 10:10 – 10:30 **O17:** Marcel A. H. Moelands (Utrecht University, The Netherlands): Homogeneous oxidation catalysis by proline-based manganese complexes
- 10:30 – 11:00 Coffee Break

Chairperson: Henrique Teles

- 11:00 – 11:50 **PL8:** Tsutomu Katsuki (Kyushu University, Japan): Development of Atom-Efficient Asymmetric Oxygen Atom Transfer Reaction
- 11:50 -12:20 **IL11:** Andreas Schmid (Laboratory of Chemical Biotechnology, Dortmund, Germany): Specific oxyfunctionalizations of hydrocarbons by oxygenases: biocatalyst design and efficiency
- 12:20 – 12:40 **O18:** Isabel Arends (Delft University of Technology, The Netherlands): Design and applications of oxidases and peroxidases: cofactor-independent enzymes as oxidative biocatalysts
- 12:40 – 13:00 **O19:** Uwe Beifuss (University of Hohenheim, Germany): Heterocycles via laccase catalyzed domino reactions with O<sub>2</sub> as the oxidant
- 13:00 – 15:00 Lunch

Chairperson: Miguel Costas

- 15:00 – 15:50 **PL9:** Luigi Casella (Università di Pavia, Italy): Tyrosinase: Mechanism of Dioxygen Activation, Intermediates, and New Reactivities
- 15:50 – 16:10 **O20:** Wolfgang Kroutil (University of Graz, Austria): Studies on the enzymatic cleavage of C=C bonds

- 16:10 – 16:30      **O21:** Vlada B. Urlacher (University of Stuttgart, Germany):  
Engineering of cytochrome P450 monooxygenases for selective  
oxidation of terpenes
- 16:30 – 17:00      **IL12:** Ulrich Schwaneberg (Jacobs University Bremen,  
Germany): Cosolvent effects on oxygenation activity of  
cytochrome P450 BM-3
- 18:30                Social Dinner

## Friday July 25<sup>th</sup>

Chairperson: T. Daniel P. Stack

- 9:00 – 9:30 **IL13:** Jeremy N. Harvey (University of Bristol, UK): QM/MM Exploration of reactivity and selectivity in cytochrome P450
- 9:30 – 9:50 **O22:** Sam P. De Visser (University of Manchester, UK): Differences and comparisons of oxygen activation by heme and nonheme enzymes and biomimetics as obtained from theoretical modelling
- 9:50 – 10:10 **O23:** George Britovsek (Imperial College London, UK): Towards catalytic alkane oxidation via O<sub>2</sub> insertion into platinum methyl bonds
- 10:10 - 10:40 **IL14:** Shannon S. Stahl (University of Wisconsin-Madison, USA): Copper-catalyzed organometallic oxidase reactions
- 10:40 – 11:10 Coffee Break

Chairperson: Brian R. James

- 11:10 – 11:30 **O24:** Csaba Varszegi (Katholieke Universiteit Leuven, Belgium): A catalytic aziridine synthesis from styrenes and ammonia
- 11:30 – 11:50 **O25:** Mark James Muldoon (Queen's University Belfast, UK): Palladium catalysed aerobic oxidation reactions in carbon dioxide-expanded liquids
- 11:50 – 12:10 **O26:** Tai Chu Lau (City University of Hong Kong, China): Efficient catalytic oxidation of alkanes by Lewis acid / [Os<sup>VI</sup>(N)Cl<sub>4</sub>]- using peroxides as terminal oxidants. Evidence for a metal-based active intermediate
- 12:10 – 13:00 **PL10:** Roger A. Sheldon (Delft University of Technology, The Netherlands): Activation of Dioxygen and Homogeneous Catalytic Oxidation: Retrospect and Prospect
- 13:00 Closing Remarks