

Program iCHAT 2022

Scientific Sessions	June 26	Hotel Villa Vecchia
	June 27-30	Villa Mondragone – Sala degli Svizzeri
Poster Session	June 29	Villa Mondragone
Lunches	June 27-30	Villa Mondragone – Portico del Vasanzio

Sunday, June 26

12:00-16:00 **Registration** (Hotel Villa Vecchia)

16:00-16:30 **Welcome Coffee**

16:30-16:45 **Opening Remarks**

Chair: Doron Pappo

16:45-17:35 **IL1 Miquel Costas**
Site and Enantioselective Oxidation of Strong C–H bonds with Bioinspired Catalysts

17:35-18:25 **IL2 Davide Ravelli**
Hydrogen Atom Transfer for Synthetic Applications: Decatungstate Photocatalysis and Beyond

18:25-18:55 **OL1 Fabrice Dénès**
Radical Cascade involving Highly Regioselective Hydrogen Atom Transfers

20:00 **Welcome Cocktail**

Monday, June 27

Chair: Nadia G. Leonard

9:00-9:50 **IL3 Andrew S. Borovik**
The Role of Metal-Oxido Complexes in C–H Bond Activation

9:50-10:40 **IL4 Doron Pappo**
Enantioselective Oxidative Phenol Coupling by Chiral Multicoordinated Iron Complexes

10:40-11:10 **OL2 Andrea Álvarez**
Exploring the Intramolecular Chemistry of Iron(V)-oxo-carboxylato Species

11:10-11:40 *Coffee Break*

Chair: Erik J. Alexanian

11:40-12:30 **IL5 David A. Nagib**
Remote, Double, and Enantioselective C–H Functionalizations via Radical Chaperones

12:30-13:00 **OL3 Andrea Palone**
Enantioselective Aliphatic C–H Hydroxylation with Biologically Inspired Oxidation Catalysts

13.00-14.30 *Lunch*

Chair: Martin Klussmann

14:30-15:20 **IL6 Erik J. Alexanian**
New Strategies for Hydrocarbon Functionalization

15:20-15:50 **OL4 Alastair J. McMillan**
Controlling HAT Selectivity: C(sp³)–H Chlorinations and [Co]-Catalysed contra-Thermodynamic Eliminations

15:50-16:20 **OL5 Daniele Mazzeola**
Rapid and Direct Photocatalytic C(sp³)–H Acylation and Arylation in Flow

16:20-16:50 *Coffee Break*

Chair: Cristina Nevado

16:50-17:40 **IL7 Daniele Leonori**
Hydrogen-Atom Transfer in Halogen-Atom and Group Transfer Chemistry

17:40-18:30 **IL8 Paolo Melchiorre**
Photochemistry & Organocatalysis: New Radical Opportunities

19.30 *Wine Tasting @ L'Olivella*

Tuesday, June 28

Chair: Helmut Schwarz

9:00-9:50 **IL9 Joan B. Broderick**
Radical Initiation in Radical SAM Enzymes

9:50-10:40 **IL10 Mark S. Taylor**
Hydrogen Atom Transfer Reactions of Carbohydrate Derivatives

10:40-11:10 **OL6 Marko Hanževački**
Activation of Glycyl Radical Enzymes: Insights from Multiscale Modeling

11:10-11:40 **Coffee Break**

Chair: Andrea Sartorel

11:40-12:30 **IL11 Julio Lloret-Fillol**
Light-Driven Reduction of Olefins by Cobalt Complexes

12:30-13:00 **OL7 Andrea Basso**
Solventylation Reactions: a New Approach for the Functionalization of Alkenes

13:00-14:30 **Lunch**

Chair: Marcella Bonchio

14:30-15:20 **IL12 Cristina Nevado**
HAT Processes in Radical Cascade Multicomponent Reactions

15:20-15:50 **OL8 Giorgio Olivo**
Supramolecular Control of Selectivity in Aliphatic C–H Oxidation

15:50-16:20 **OL9 Thomas Rigotti**
Lewis Acid Mediated Photochemical Hydrogen Atom Transfer: from Theoretical and Spectroscopical Studies of the Benzaldehyde-BCl₃ Complex to Synthetic Applications

16:20-16:50 **Coffee Break**

Chair: Maurizio Fagnoni

16:50-17:40 **IL13 Luca Valgimigli**
The Antioxidant Chemistry of Quinones / HOO• Catalytic Systems

17:40-18:10 **OL10 Manfredi Caruso**
N-Hydroxyphthalimide Role in Aerobic Oxidations: Homogeneous versus Heterogeneous Catalysis

18:10-18:40 **OL11 Giorgio Capocasa**
More than the Sum of its Parts: Combining UV-Vis and XAS to Investigate Reaction Mechanisms

20:00 **Free Dinner**

Wednesday, June 29

Chair: Julio Lloret-Fillol

- 9:00-9:50 **IL14 Marcella Bonchio**
Photosystem II-inspired Supramolecular “Quantasomes” for Artificial Photosynthesis
- 9:50-10:40 **IL15 Leif Hammarström**
Proton-Coupled Electronic Processes in Molecular Triads
- 10:40-11:10 **OL12 Guilherme L. Tripodi**
The Mass Spectrometry Factory: An Fe^{IV}O Perspective
- 11:10-11:40 *Coffee Break*

Chair: Andrea Basso

- 11:40-12:30 **IL16 Hendrik Zipse**
Oxidation of 5-Methylcytosine and Derivatives
- 12:30-13:00 **OL13 Julia Turner**
Hydrogen Abstraction in Carbohydrates: A Computational Study of the Effects of Substitution and Configuration on Free Energies of Activation
- 13:00-14:30 *Lunch*

Chair: Fabrice Dénès

- 14:30-15:20 **IL17 Jie Wu**
Neutral Eosin Y as Efficient Photo Hydrogen Atom Transfer Catalyst
- 15:20-15:50 **OL14 Luca Capaldo**
Continuous-flow as an Enabling Technology for Photocatalyzed Hydrogen Atom Transfer
- 15:50-18:30 *Coffee Break and Poster Session*
- 20.00 *Conference Dinner @ Ristorante Cacciani*

Thursday, June 30

Chair: **Jie Wu**

- 9:00-9:50 **IL18 Gonzalo Cosa**
Harnessing Photoinduced Electron Transfer Towards Development in Fluorescence Imaging
- 9:50-10:40 **IL19 Nadia G. Leonard**
Cationic Effects at Manganese Nitride and Vanadium Oxo Complexes and Applications to Hydrogen Atom Transfer Reactivity
- 10:40-11:10 **OL15 Derek Rice**
Evaluating Fe(IV)-Oxo Two-State Reactivity using Resonant Inelastic X-ray Scattering and Magnetic Circular Dichroism
- 11:10-11:40 **Coffee Break**

Chair: **Davide Ravelli**

- 11:40-12:10 **OL16 Niklas von Wolff**
Towards the Electrification of Metal-Ligand Cooperative Catalysts
- 12:10-12:40 **OL17 Andrea Sartorel**
Proton-coupled Electron Transfer Reactivity in Artificial Photosynthetic Schemes
- 12:40-12:50 **Concluding Remarks**
- 12:50 **Lunch**