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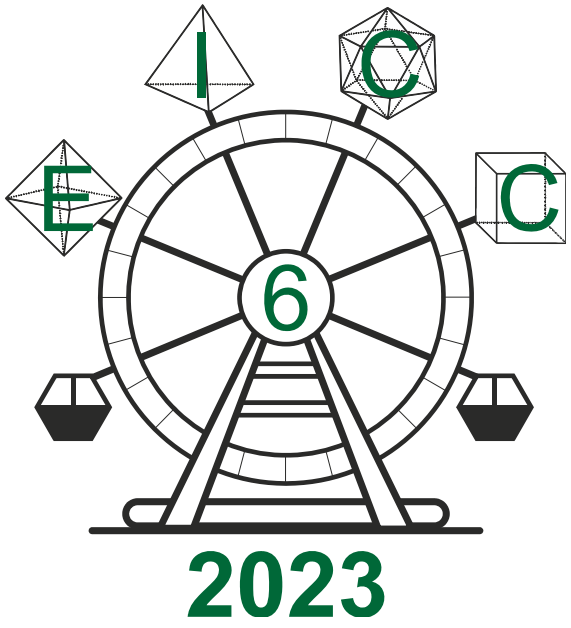

September 3 – 7, 2023

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WELCOME FROM THE CHAIRMEN OF THE 6TH EUCHEMS INORGANIC CHEMISTRY CONFERENCE

Dear Colleagues,

We wish to cordially welcome you to the 6th EuChemS Inorganic Chemistry Conference 2023 at the TU Wien. This series of meetings has been initiated in 2011 and since then developed to a true European event organized every two years. The 6th EICC covers all aspects of inorganic chemistry with special focus on coordination & supramolecular chemistry, organometallic chemistry & catalysis, magnetochemistry, energy & photochemistry, green & bioinorganic chemistry, inorganic materials & nanoparticles, nuclear chemistry and theoretical inorganic chemistry.

Ideally located in the center of Europe, Vienna has a long-standing tradition as a major conference site since the "Congress of Vienna" in 1815. Its unique atmosphere will provide inspiration for a fruitful scientific meeting, and the participants will have ample time to enjoy a wealth of culture and historical places in and around Austria's capital city.

We hope that you find the conference interesting and stimulating and wish you a pleasant stay in Vienna.

Sincerely,

Peter Weinberger and Karl Kirchner
Chairmen of 6th EICC

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The conference is organized by the Institute of Applied Synthetic Chemistry at the TU Wien.

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The organizers acknowledge the support given by the TU Wien, in particular by Sabine Seidler (rector).

Sunday, September 3

15.30-17.00 Registration

Session 1
Chair: P. Weinberger

Lecture hall HS1

17.00-17.30 Opening Ceremony

17.30-18.15 **Roberta Sessoli**
PL-1 *Università degli Studi di Firenze, Italy*
"MAGNETIC MOLECULES IN QUANTUM NANOSCIENCE: POTENTIAL AND CHALLENGES"

18.30-19.30 Independend move to the Town Hall

19.30-21.30 Welcome Mixer

Monday, September 4

08.30-09.00 Registration

Session 2
Chair: G. Steinhauser

Lecture hall HS1

09.00-09.45 **Erwin Reisner**
PL-2 *University of Cambridge, UK*
"SOLAR PANELS FOR LIGHT-TO-CHEMICAL CONVERSION"

09.45-10.15 **Alenka Ristić**
IL-1 *National Institute of Chemistry, Slovenia*
"DEVELOPMENT OF ADVANCED MATERIALS FOR ADSORPTION THERMAL BATTERY"

10.15-10.45 **Eva Hevia**
IL-2 *University of Bern, Switzerland*
"HARNESSING COORDINATION AND COOPERATIVE EFFECTS TO TAME ORGANOSODIUM CHEMISTRY"

10.45-11.15 Coffee break

Lecture hall HS1

Parallel Session A - Catalysis 1
Chair: A. Phillips

11.15-11.35 **Estefanía Díaz-López**
OP-1 *Universitat Autònoma de Barcelona, Spain*
"KINETIC ANALYSIS OF DRY REFORMING OF METHANE CATALYZED BY Rh (111)"

11.35-11.55 **Luka Suhadolnik**
OP-2 *University of Trieste, Italy*
"ANODIZED ALLOYS AS HIGHLY ACTIVE OXYGEN EVOLUTION REACTION ELECTROCATALYSTS"

11.55-12.15 **Andrew Swarts**
OP-3 *University of the Witwatersrand, South Africa*
"HIGHLY EFFICIENT TRANSFER HYDROGENATION OF ALKENES WITH AMMONIA BORANE MEDIATED BY A SIMPLE Ni(II) CATALYST SYSTEM"

12.15-12.35 **Niklas von Wolff**
OP-4 *Université Paris Cité, France*
"TOWARDS THE ELECTRIFICATION OF METAL-LIGAND COOPERATIVE CATALYSTS"

Lecture hall HS8

Parallel Session B - Theoretical Inorganic Chemistry 1
Chair: P.-O. Norrby

11.15-11.35 **Bettina Lier**
OP-21 *University of Natural Resources and Applied Life Sciences, Austria*
"SIMULATION OF METAL COORDINATION COMPLEXES WITH THE BuRNN APPROACH"

11.35-11.55 **Radu A. Talmazan**
OP-22 *TU Wien, Austria*
"TACKLING DYNAMICS AND SOLVATION IN TRANSITION-METAL CATALYSIS"

11.55-12.15 **Anna Vidal-López**
OP-23 *Autonomous University of Barcelona, Spain*
"CATALYTIC ACTIVITY OF Cu/Mo_2CT_x: HYDROGENATION OF CO_2 AND CO TO METHANOL"

12.15-12.35 **Felipe Fantuzzi**
OP-24 *University of Kent, U.K.*
"ELECTRONIC STRUCTURE, BONDING AND REACTIVITY OF EMERGING BORON-BASED SYSTEMS: INSIGHTS FROM THEORY"

Parallel Session C - Coordination Chemistry 1
Chair: S. Suman

Lecture hall HS6

11.15-11.35 **Miljan Ćorović**
OP-29 *University of Graz, Austria*
"THE REDUCTION OF TUNGSTEN(VI) DIOXIDO COMPLEXES OPENS THE DOOR FOR NEW REACTIVITIES"

11.35-11.55 **Errikos Kounalis**
OP-30 *Utrecht University, The Netherlands*
"A KINETICALLY TRAPPED $[TiCl_3]^+$ CATION: COORDINATION AND REACTIVITY"

11.55-12.15 **Małgorzata Zienkiewicz-Machnik**
OP-31 *Polish Academy of Science, Poland*
"COMBINED EXPERIMENTAL AND THEORETICAL STUDIES OF Cu(II) AND Co(II) CATIONIC-ANIONIC COMPLEXES WITH N-SCORPIONATE LIGAND - SIMILAR STRUCTURES BUT DIFFERENT REACTIVITY"

12.15-12.35 **Rasika Dias**
OP-32 *The University of Texas at Arlington, USA*
"COPPER COMPLEXES OF HIGHLY FLUORINATED PYRAZOLATES"

12.35-14.00 Lunch

Session 3
Chair: P. Weinberger

Lecture hall HS1

14.00-14.45 **Eugenio Coronado**
PL-3 *University of Valencia, Spain*
"MAGNETIC MOLECULES IN 2D MATERIALS"

14.45-15.15 **Marko Hapke**
IL-3 *Johannes Kepler University Linz, Austria*
"CYCLOADDITION REACTIONS WITH MANGANESE AND COBALT PRECATALYSTS: CATALYTIC TWINS?"

15.15-15.45 **Lubomír Rulíšek**
IL-4 *Czech Academy of Sciences, Czech Republic*
"ELUCIDATING REACTION MECHANISMS OF COUPLED BINUCLEAR COPPER ENZYMES BY CORRELATING QM/MM CALCULATIONS AND SPECTROSCOPY"

15.45-16.15 Coffee break

Lecture hall HS1

Parallel Session D - Catalysis 2
Chair: M. Hapke

16.15-16.35 **Roel Bienenmann**
OP-5 *Utrecht University, The Netherlands*
"MECHANISTIC INVESTIGATION INTO COPPER(I) HYDRIDE CATALYZED FORMIC ACID DEHYDROGENATION"

16.35-16.55 **Carla D. Nunes**
OP-6 *Universidade de Lisboa, Portugal*
"CATALYTIC OXIDATIVE DESULFURIZATION FOR A CLEANER ENVIRONMENT"

16.55-17.15 **Rosa Llusar**
OP-7 *Universitat Jaume I, Spain*
"CATALYTIC HYDROGENATION AND DEHYDROGENATION REACTION MECHANISMS MEDIATED BY MOLYBDENUM SULFIDE CLUSTERS"

17.15-17.35 **Hugo Lapa**
OP-8 *Universidade de Lisboa, Portugal*
"NEW RUTHENIUM AND COPPER COMPLEXES AS CATALYSTS OF C-C COUPLING REACTIONS OF ALKYNES"

Lecture hall HS8

Parallel Session E - Theoretical Inorganic Chemistry 2
Chair: L. Rulíšek

16.15-16.35 **Jordi Cirera**
OP-25 *Universitat de Barcelona, Spain*
"EXPLORING THE LIGAND CHEMICAL SPACE IN SPIN-CROSSOVER MOLECULES WITH ELECTRONIC STRUCTURE METHODS"

16.35-16.55 **Martin Breza**
OP-26 *Slovak University of Technology, Slovakia*
"JAHN-TELLER EFFECT IN DIMETHYL AMINO PHENYL SUBSTITUTED SILVER PHTHALOCYANINE "

16.55-17.15 **Jorge Echeverría**
OP-27 *Universidad de Zaragoza, Spain*
"TRANSFORMING METHYL GROUPS INTO LEWIS BASES WITH MAIN GROUP METALS"

17.15-17.35 **Maria Jaworska**
OP-28 *University of Silesia, Poland*
"INTERACTION OF PALLADIUM PORPHYRIN WITH DIOXYGEN MOLECULE. THE PERSPECTIVE FROM THEORETICAL CALCULATIONS"

Parallel Session F - Nuclear Chemistry
Chair: U. Abram

Lecture hall HS6

16.15-16.35 **Erik Strub**
OP-41 *University of Cologne, Germany*
"PERTECHNETATE TALES: SUPERACIDS, NEW PERTECHNETATE FAMILY MEMBERS, AND THE COLOUR OF PERTECHNETIC ACID "

16.35-16.55 **Manuel Luca Besmer**
OP-42 *University of Zurich, Switzerland*
"^{99}Tc-PNP PINCER COMPLEXES INTERACTING WITH SMALL MOLECULES"

16.55-17.15 **Raphael Lengacher**
OP-43 *Stony Brook University, USA*
"CHERENKOV-MEDIATED EXCITATION OF DISCRETE EUROPIUM PROBES FOR IN VIVO LUMINESCENCE IMAGING FOR INTRAOPERATIVE TUMOR RESECTION"

17.15-17.35 **Andreas Roodt**
OP-44 *University of the Free State, South Africa*
"STRUCTURE/ (RE)ACTIVITY RELATIONSHIPS IN RADIOPHARMACEUTICAL COORDINATION CHEMISTRY: IS IT NECESSARY?"

17.50-19.50 Poster Session 1 with Drinks&Snacks

18.15-19.45 Advisory Board Meeting

Tuesday, September 5

Lecture hall HS1

Session 4
Chair: K. Kirchner

09.00-09.45 **Matthias Beller**
PL-4 *Leibniz Institute for Catalysis e.V., Germany*
"WITH A LITTLE HELP FROM MY FRIENDS - THE IMPORTANCE OF LIGANDS AND SUPPORTS FOR SUSTAINABLE CATALYSIS"

09.45-10.15 **Maja Gruden**
IL-5 *University of Belgrade, Serbia*
"THE ROLE OF DFT IN CHARACTERIZATION OF COORDINATION COMPOUNDS: OPPORTUNITIES AND CHALLENGES"

10.15-10.45 **Marius Andruh**
IL-6 *Romanian Academy, Romania*
"METAL-RADICAL COMPLEXES IN MOLECULAR MAGNETISM. NEW SYNTHETIC APPROACHES"

10.45-11.15 Coffee break

Lecture hall HS1

Parallel Session G - Catalysis 3
Chair: G. Seisenbaeva

11.15-11.35 **Thomas Lohmiller**
OP-9 *Humboldt Universität zu Berlin, Germany*
"SMALL MOLECULE ACTIVATION AT TRANSITION METAL CENTERS STUDIED BY EPR: OXYGEN ACTIVATION AT BIOMIMETIC DINUCLEAR SITES AND CO_2 REDUCTION BY A Co COMPLEX"

11.35-11.55 **Heiko Schratzberger**
OP-10 *TU Wien, Austria*
"TRANSFER-SEMIHYDROGENATION OF ALKYNES CATALYZED BY AN IRON(II) PCP DICARBONYL ALKYL COMPLEX"

11.55-12.15 **Alexander Sorokin**
OP-11 *Université Lyon-1, France*
"CARBENE INSERTION INTO X-H BONDS PROMOTED BY PHTHALOCYANINE COMPLEXES"

12.15-12.35 **Andrew Phillips**
OP-12 *University College Dublin, Ireland*
"HIGHLY STABLE DIIMINE SILVER(I) CATALYSTS THAT INCORPORATE CO_2 INTO ALKYNES FRAMEWORKS"

Lecture hall HS8

Parallel Session H - Organometallic Chemistry 1
Chair: E. Hevia

11.15-11.35 **Malte Sellin**
OP-49 *Albert-Ludwigs-Universität Freiburg, Germany*
"THE ART OF SELECTIVELY REMOVING ELECTRONS FROM ORGANIC MOLECULES AND METAL COMPLEXES IN CONDENSED PHASE"

11.35-11.55 **Nikolaus Gorgas**
OP-50 *TU Wien, Austria*
"COOPERATIVE C-H BOND ACTIVATION BY A LOW-SPIN d^6 IRON-ALUMINIUM COMPLEX"

11.55-12.15 **Doris Kunz**
OP-51 *University of Tübingen, Germany*
"ELUCIDATING THE REACTIVITY OF EARLY TRANSITION METAL COMPLEXES BEARING ELECTRON POOR Cp LIGANDS"

12.15-12.35 **Vladimir Lee**
OP-52 *University of Tsukuba, Japan*
"GROUP 4 METAL SILYLIDENES AND GERMYLIDENES"

Lecture hall HS6

Parallel Session I - Coordination Chemistry 2
Chair: M. Gruden

11.15-11.35 **Danielle Runacres**
OP-33 *University of Southampton, UK*
"^{18}F-RADIOLABELING OF MAIN GROUP AND TRANSITION METAL BASED CHELATES FOR PET IMAGING APPLICATIONS"

11.35-11.55 **Guillem Aromí**
OP-34 *Universitat de Barcelona, Spain*
"SYNTHESIS, MAGNETISM AND PHOTOPHYSICS OF HETEROMETALLIC LANTHANIDE COORDINATION COMPLEXES"

11.55-12.15 **Maciej Wyczesany**
OP-35 *Jagiellonian University, Poland*
"POLYCYANIDOPLATINATE MOLECULAR BUILDING BLOCKS FOR THE MODULATION OF Eu(III)- AND Tb(III)-BASED OPTICAL THERMOMETRY"

12.15-12.35 **Johann Hlina**
OP-36 *University of Graz, Austria*
"HETEROBIMETALLIC COMPLEXES OF RARE-EARTH AND LATE TRANSITION METALS"

12.35-14.00 Lunch

Session 5
Chair: G. Steinhauser

Lecture hall HS1

14.00-14.45 **Marc Fontecave**
PL-5 *Collège de France, France*
"FROM CO_2 TO FUELS: BIOINSPIRED METAL CATALYSTS "

14.45-15.15 **Thomas Klapötke**
IL-7 *LMU Munich, Germany*
"TKX-50 - A NEW HIGH EXPLOSIVE, DEVELOPED AT LMU MUNICH"

15.15-15.45 **Marcel Swart**
IL-8 *Universitat de Girona, Spain*
"COMPUTATIONAL TOOLS FOR DESIGNING NEW CATALYSTS: OPPORTUNITIES AND CHALLENGES"

15.45-16.15 Coffee break

Parallel Session J - Magnetochemistry
Chair: M. Andruh

Lecture hall HS1

16.15-16.35 **Livia Getzner**
OP-45 *Université de Toulouse, France*
"SPIN CROSSOVER COUPLED WITH AN ELECTRON TRANSFER IN HOFMANN-TYPE COORDINATION POLYMERS"

16.35-16.55 **Willi Zeni**
OP-46 *TU Wien, Austria*
"HOST-GUEST CHEMISTRY IN SECOND GENERATION SPINSWITCHABLE HOFMANN TYPE NETWORKS: LARGER PORES FOR LARGER GUESTS"

16.55-17.15 **Szymon Chorazy**
OP-47 *Jagiellonian University, Poland*
"FORMATION OF TERBIUM(III) SINGLE-MOLECULE MAGNETS IN A RIGID HEXACYANIDOMETALLATE-BASED COORDINATION NETWORK"

17.15-17.35 **Christian Dirk Buch**
OP-48 *University of Copenhagen, Denmark*
"A CHEMIST'S TOOLBOX TO TUNE 4F MOLECULAR QUBITS"

Parallel Session K - Organometallic Chemistry 2
Chair: A. Ristić

Lecture hall HS8

16.15-16.35 **Clara Schweinzer**
OP-53 *ETH Zürich, Switzerland*
"STRUCTURAL MODIFICATIONS IN THE CARBON SPHERE OF A DIRHODIUM COMPLEX"

16.35-16.55 **Hugo Valdés**
OP-54 *Universitat de Girona, Spain*
"NOVEL $C_{(NHC)}CC_{(NHC)}$-NHC GOLD PINCER COMPLEXES AND STUDY OF THEIR CATALYTIC ACTIVITIES"

16.55-17.15 **Rudolf Pietschnig**
OP-55 *University of Kassel, Germany*
"HETEROCARBENES EMBEDDED INTO STEREOCHEMICALLY DEFINED PHOSPHA-FERROCENOPHANES"

17.15-17.35 **Susanne Rupf**
OP-56 *Freie Universität Berlin, Germany*
"SYNTHESIS OF A FERROCENE DECA- AND UNDECACATION"

Parallel Session L - Energy /Photochemistry
Chair: M. Swart

Lecture hall HS6

16.15-16.35 **Phebe H. van Langevelde**
OP-57 *Leiden University, The Netherlands*
"MOLECULAR COPPER CATALYSTS FOR SUSTAINABLE AND EFFICIENT H_2O_2 PRODUCTION"

16.35-16.55 **Nora S. Grundmann**
OP-58 *University of Zurich, Switzerland*
"STRUCTURE-ACTIVITY RELATIONSHIP IN COBALT POLYPYRIDYL WATER REDUCING CATALYSTS - THE QUEST FOR REDUCED OVERPOTENTIALS"

16.55-17.15 **Frédéric Dumur**
OP-59 *Aix-Marseille Université, France*
"MECHANOSYNTHESIS: GREEN CHEMISTRY APPLIED TO THE DESIGN OF COPPER-BASED PHOTOINITIATORS OF POLYMERIZATION"

17.15-17.35 **Laura Sánchez Muñoz**
OP-60 *Universitat de Barcelona, Spain*
"COMPUTATIONAL MODELLING OF Eu^{III}-BASED DOWN-SHIFTING SPECTRAL CONVERTERS FOR NOVEL SOLAR CELL TECHNOLOGIES"

17.50-19.50 Poster Session 2 with Drinks&Snacks

Wednesday, September 6

Lecture hall HS1

Session 6
Chair: K. Kirchner

09.00-09.45 **Joost N.H. Reek**
PL-6 *University of Amsterdam, The Netherlands*
"CATALYSIS FOR THE ASSEMBLY OF M_nL_{2n} NANOSPHERES AND THE APPLICATION OF M_nL_{2n} NANOSPHERES IN CATALYSIS"

09.45-10.15 **Ulrich Abram**
IL-9 *Freie Universität Berlin, Germany*
"TECHNETIUM: BOON AND BANE - MORE CHEMISTRY IS REQUIRED"

10.15-10.45 **Nadia Mösch-Zanetti**
IL-10 *Karl-Franzens-University of Graz, Austria*
"FROM NATURE TO ORGANOMETALLIC CHEMISTRY - INSIGHTS INTO THE MECHANISM OF ACETYLENE HYDRATASE"

10.45-11.15 Coffee break

Lecture hall HS1

Parallel Session M - Catalysis 4
Chair: G. Morgan

11.15-11.35 **Dan Meyerstein**
OP-13 *Ariel University, Israel*
"THE ROLES OF HCO_3^-/CO_3^{2-} IN CATALYTIC OXIDATION PROCESSES"

11.35-11.55 **Michel Sigrist**
OP-14 *Université de Strasbourg, France*
"ISO-SELECTIVE HYDROFORMYLATION OF PROPYLENE BY IODIDE-ASSISTED PALLADIUM-CATALYSIS"

11.55-12.15 **Murielle F. Delley**
OP-15 *University of Basel, Switzerland*
"CATALYSIS BY INORGANIC MATERIALS: CONTROL AT THE SURFACE BY TAILORED INTERFACES AND ELECTRIC FIELDS"

12.15-12.35 **Martin Smith**
OP-16 *Loughborough University, United Kingdom*
"REVERSIBLE P-P BOND CLEAVAGE OF METAL COORDINATED DIPHOSPHANES"

Lecture hall HS8

Parallel Session N - Bioinorganic Chemistry
Chair: G. Aromí

11.15-11.35 **Sara Ida Mozzi**
OP-61 *University of Göttingen, Germany*
"MODELLING CO DEHYDROGENASES: DINICKEL(II) μ-OH PLATFORM FOR CO OXIDATION TO CO_2"

11.35-11.55 **Liam Grunwald**
OP-62 *ETH Zürich, Switzerland*
"EXPLOITING EXTREMELY VARIABLE REDOX CHEMISTRY AT CUBANE-TYPE IRON-SULFUR CLUSTERS"

11.55-12.15 **Silene Engbers**
OP-63 *University of Groningen, The Netherlands*
"IRON(III) Π-DICATIONS: A KEY INTERMEDIATE TOWARDS BIOINSPIRED UMPOLUNG OF CHLORIDE"

12.15-12.35 **Maria Drosou**
OP-64 *Max-Planck-Institut für Kohleforschung, Germany*
"PHOTOSYNTHETIC WATER OXIDATION: NEW INSIGHTS FROM X-RAY SPECTROSCOPY"

Lecture hall HS6

Parallel Session O - Coordination Chemistry 3
Chair: N. Mösch-Zenetti

11.15-11.35 **Ting-Yi Chen**
OP-37 *Georg-August-Universität, Germany*
"A LOW-COORDINATE N_2-BRIDGED DICOBALT(I) COMPLEX WITH NON-AUFBAU ELECTRONIC GROUND STATE"

11.35-11.55 **James N. McPherson**
OP-38 *Technical University of Denmark, Denmark*
"METAL-ORGANIC FRAMEWORKS WITH ZERO-VALENT METAL NODES"

11.55-12.15 **Nadiia Gumerova**
OP-39 *University of Vienna, Austria*
"SPECIATION ATLAS OF POLYOXOMETALATES IN AQUEOUS SOLUTIONS"

12.15-12.35 **Victoria Greenacre**
OP-40 *University of Southampton, UK*
"COORDINATION CHEMISTRY OF $WSCl_4$ AND $WSeCl_4$: TOWARDS PRECURSORS FOR WE_2 THIN FILM DEPOSITION"

12.35-14.00 Lunch

Session 7
Chair: M. Podewitz

Lecture hall HS1

14.00-14.45 **Roger Alberto**
PL-7 *University of Zurich, Switzerland*
"ADVANCES IN TECHNETIUM AND RHENIUM CHEMISTRY: STILL RELEVANT FOR MOLECULAR IMAGING?"

14.45-15.15 **Karol Grela**
IL-11 *University of Warsaw, Poland*
"PLAYING WITH C-C MULTIPLE BONDS: FROM OLEFIN METATHESIS TO ALKENE AND ALKYNE HYDROGENATION"

15.15-15.45 **Mats Tilset**
IL-12 *University of Oslo, Norway*
"TRANS EFFECTS IN GOLD(III) CHEMISTRY: IMPLICATIONS FOR STRUCTURE, REACTIVITY, AND CATALYSIS"

15.45-16.15 Coffee break

Parallel Session P - Catalysis 5
Chair: M. Tilset

Lecture hall HS1

16.15-16.35 **Yongjian Lai**
OP-17 *Université de Toulouse, France*
"FROM PSM MODIFICATION ON IRON-TRIAZOLE SPIN CROSSOVER COMPLEXES TO THEIR USE IN CATALYSIS"

16.35-16.55 **Albert Ruggi**
OP-18 *Université de Fribourg, Switzerland*
"A TALE OF TWO METALS: SWITCHING SELECTIVITY TOWARDS CO_2 REDUCTION IN HEPTACOORDINATE COMPLEXES"

16.55-17.15 **Sigridur Suman**
OP-19 *University of Iceland, Iceland*
"COBALT CATALYZED CO_2 INCORPORATION INTO CYCLIC CARBONATES"

17.15-17.35 **Martin Hejda**
OP-20 *University of Pardubice, Czech Republic*
"UNSEEN REDOX E-H BOND ACTIVATIONS USING TELLURIUM-CENTERED LEWIS ACID"

Parallel Session Q - Inorganic Materials
Chair: R. Pietschnig

Lecture hall HS8

16.15-16.35 **Gulaim Seisenbaeva**
OP-65 *Swedish University of Agricultural Sciences, Sweden*
"ADVANCED ADSORBENTS AND BIOCATALYSTS FOR ENVIRONMENTAL APPLICATIONS"

16.35-16.55 **Lucie Routaboul**
OP-66 *Laboratory of Coordination Chemistry, France*
"POST-SYNTHETIC MODIFICATION MECHANISM FOR 1-D SPIN CROSSOVER COORDINATION POLYMERS"

16.55-17.15 **Lorenzo Lisuzzo**
OP-67 *Università degli Studi di Palermo, Italy*
"COMPUTATIONAL AND EXPERIMENTAL STUDIES OF HALLOYSITE MODIFIED SURFACES FOR EFFICIENT FUNCTIONALIZATION"

17.15-17.35 **Jan Gertenbach**
OP-68 *Malvern Panalytical B. V., The Netherlands*
"COMPLEX PHASE DIAGRAM IN $NaSrPO_4$"

Parallel Session R - Nanoparticles /Supramolecular Chemistry
Chair: Chr. Mitsopoulou

Lecture hall HS6

16.15-16.35 **Lucy Browne**
OP-69 *University of Oxford, UK*
"CONTROLLED BIOCATALYTIC SYNTHESIS OF METAL NANOPARTICLE-ENZYME HYBRIDS: DEMONSTRATION FOR CATALYTIC H_2-DRIVEN NADH OR FLAVIN RECYCLING"

16.35-16.55 **Troy Breijaert**
OP-70 *Swedish University of Agricultural Sciences, Sweden*
"METAL OXIDE NANOPARTICLES FOR DELAYED DRUG RELEASE IN WOUND DRESSING MATERIALS"

16.55-17.15 **De-Liang Long**
OP-71 *University of Glasgow, United Kingdom*
"FUNCTIONALIZATION OF MOLYBDENUM BLUE POLYOXOMETALATES WITH AMINO ACIDS AND PEPTIDES "

17.15-17.35 **Nerea Álvarez-Llorente**
OP-72 *Universidad de Valladolid, Spain*
"Au(I) BIS-ACETYLIDES WITH DIPHOSPHINE BRIDGING LIGANDS AS MOLECULAR TWEEZERS FOR FULLERENES"

18.15-19.08 Tramway transfer

19.00-22.00 Conference Dinner

Thursday, September 7

Lecture hall HS1

Session 8
Chair: P. Weinberger

10.00-10.45 **Christine Joy McKenzie**
PL-8 *University of Southern Denmark, Denmark*
"BIOMIMETIC OXIDATION REACTIONS BY IRON COMPLEXES"

10.45-11.15 **Christiana Mitsopoulou**
IL-13 *National and Kapodistrian University of Athens, Greece*
"LIGHT-INDUCED HYDROGEN PRODUCTION FROM WATER USING NICKEL(II) CATALYSTS: THE ROLE OF THE NON-INNOCENT LIGANDS, THE REACTION MECHANISM, AND THE NUCLEARITY IN THE CATALYTIC EFFICIENCY"

11.15-11.45 **Per-Ola Norrby**
IL-14 *AstraZeneca, Sweden*
"PREDICTING REACTION SELECTIVITY"

11.45-12.15 Coffee break

Lecture hall HS1

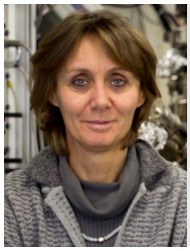
Session 9
Chair: M. Podewitz

12.15-12.45 **Grace Morgan**
IL-15 *University College Dublin, Ireland*
"SPIN STATE SWITCHING IN NON-CENTROSYMMETRIC CRYSTALS"

12.45-13.30 **Leticia Gonzalez**
PL-9 *University of Vienna, Austria*
"CALCULATING LIFETIMES IN PHOTOACTIVE TRANSITION METAL COMPLEXES"

13.30-14.00 Closing Ceremony

Plenary Lectures

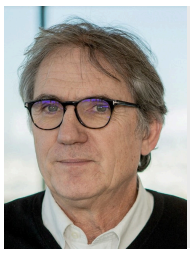


Roberta **Sessoli** **PL-1**
Università degli Studi di Firenze, Firenze, Italy
MAGNETIC MOLECULES IN QUANTUM NANOSCIENCE: POTENTIAL AND CHALLENGES

Erwin **Reisner** **PL-2**
University of Cambridge, Cambridge, UK
SOLAR PANELS FOR LIGHT-TO-CHEMICAL CONVERSION

Eugenio **Coronado** **PL-3**
University of Valencia, Valencia, Spain
MAGNETIC MOLECULES IN 2D MATERIALS

Matthias **Beller** **PL-4**
Leibniz Institute for Catalysis e.V., Rostock, Germany
WITH A LITTLE HELP FROM MY FRIENDS - THE IMPORTANCE OF LIGANDS AND SUPPORTS FOR SUSTAINABLE CATALYSIS



Marc **Fontecave** **PL-5**
Collège de France, Paris, France
FROM CO_2 TO FUELS: BIOINSPIRED METAL CATALYSTS

Joost N.H. **Reek** **PL-6**
University of Amsterdam, Amsterdam, The Netherlands
CATALYSIS FOR THE ASSEMBLY OF M_nL_{2n} NANOSPHERES AND THE APPLICATION OF M_nL_{2n} NANOSPHERES IN CATALYSIS

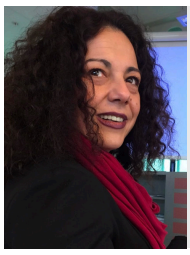
Invited Lectures

Alenka **Ristić** **IL-1**
National Institute of Chemistry, Ljubljana, Slovenia
DEVELOPMENT OF ADVANCED MATERIALS FOR ADSORPTION THERMAL BATTERY

Eva **Hevia** **IL-2**
University of Bern, Bern, Switzerland
HARNESSING COORDINATION AND COOPERATIVE EFFECTS TO TAME ORGANOSODIUM CHEMISTRY

Marko **Hapke** **IL-3**
Johannes Kepler University Linz, Linz, Austria
CYCLOADDITION REACTIONS WITH MANGANESE AND COBALT PRECATALYSTS: CATALYTIC TWINS?

Lubomír **Rulíšek** **IL-4**
Czech Academy of Sciences, Prague, Czech Republic
ELUCIDATING REACTION MECHANISMS OF COUPLED BINUCLEAR COPPER ENZYMES BY CORRELATING QM/MM CALCULATIONS AND SPECTROSCOPY



Maja **Gruden** **IL-5**
University of Belgrade, Belgrade, Serbia
THE ROLE OF DFT IN CHARACTERIZATION OF COORDINATION COMPOUNDS: OPPORTUNITIES AND CHALLENGES

Marius **Andruh** **IL-6**
Romanian Academy, Bucharest, Romania
METAL-RADICAL COMPLEXES IN MOLECULAR MAGNETISM. NEW SYNTHETIC APPROACHES

THE ROLE OF DFT IN CHARACTERIZATION OF COORDINATION COMPOUNDS: OPPORTUNITIES AND CHALLENGES

Maja Gruden[a] and Matija Zlatar[b]

[a] University of Belgrade – Faculty of Chemistry, Belgrade, Serbia
[b] University of Belgrade-ICTM, Belgrade, Serbia

In the last two decades, considerable theoretical efforts have been made to develop suitable methods for predicting and rationalizing the complicated electronic structure of TM compounds. However, the matter remains open and calculations on molecules with TM centers are still far from being straightforward. The main reason is that these calculations require a balanced treatment of both static and dynamic correlations. Furthermore, it is necessary to understand the influences of coordination number, molecular symmetry, ligand field strength, spin-orbit coupling, spin and oxidation states, redox potential, spin and charge localization, electronic degeneracies, etc. Finally, a complete understanding of the electronic structure of TM compounds and their properties requires investigations that go beyond the ground states alone, i.e., the consideration of excited states.

In this talk we will present our efforts to understand and control metal-ligand bonding based on density functional calculations, considering all its limitations. A fundamental understanding of all factors influencing the properties of a molecule is inherently related to its electronic structure. In the case of a transition metal (TM) complex, the electronic structure is determined by the number, geometry, and character (e.g., σ-donating or π*-backdonating) of its metal-ligand bonds. In addition, a variety of examples will show how experimental results and properties of coordination compounds can be rationalized using DFT calculations.

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