



16th European Biological Inorganic Chemistry Conference (EuroBIC-16)  
July, 17-21, 2022 - Grenoble (France)

Sunday - 17 July

**Belle Electrique**  
12 Esplanade Andry Farcy, 38000 Grenoble  
Tram station "Berriat -Le Magasin"

15h00-17h30

**Registration**

17h30 - 18h30

**Welcome party**

18h30 - 19h00

**Opening Ceremony**

*Chairs: Carole DUBOC - Stéphane MENAGE*

19h00 - 19h30

*Chair Eva Freisinger*

**EUROBIC Medal 2020 - Aidan MCDONALD**  
Mimicking class Ib dimanganese ribonucleotide reductase

19h30 - 20h00

**EUROBIC Medal 2020 - Kallol RAY**  
Small molecule activation at transition metal centers: structure-function correlations

8h30 - 9h20			
<b>PL1 - Elisabeth NOLAN</b>			
<b>Exploring siderophore scaffolds for antibacterial strategies</b>			
<i>Room A - Chair Roland SIGEL</i>			
	<b>Session 1 - Room B</b> <i>Chair Isabel CORREIA</i>	<b>Session 2 - Room C</b> <i>Chair Nick LE BRUN</i>	<b>Session 3 - Room D</b> <i>Chair Vincent ARTERO</i>
9:30 - 10:00	<b>KN1 ROMPEL Annette</b> <i>Interweaving disciplines to advance chemistry: applying polyoxometalates in biology</i>	<b>KN3 CIURLI Stefano</b> <i>Advances in the biochemistry of urease and related systems</i>	<b>KN5 NAM Wonwoo</b> <i>Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation Chemistry</i>
10:00 - 10:20	<b>OC1 HADJIKAKOU Sotiris</b> <i>Drug activation for the discovery and development of new targeted chemotherapeutic formulations</i>	<b>OC5 WONG Kam Bo</b> <i>Structural insights into nickel trafficking along the urease maturation pathway</i>	<b>OC9 JACKSON Timothy</b> <i>Geometric and Electronic Influences on the Reactivity of Mn(III)-hydroxo and Mn(III)-alkylperoxo Complexes</i>
10:20 - 10h40	<b>OC2 MARMION Celine</b> <i>Multi-Targeted Metallodrugs Rationally Designed to Overcome Drug Resistance</i>	<b>OC6 FURTMUELLER Paul</b> <i>Structural and mechanistic insights in dimeric chlorite dismutase - Impact of pH and the dynamics of the catalytic arginine</i>	<b>OC10 DEY Abhishek</b> <i>Nitric Oxide Reactivity with Iron Porphyrins</i>
10h40-11h10 <b>Coffee Break</b>			
	<b>Session 1 - Room B</b> <i>Chair Juan FONTECILLA-CAMPS</i>	<b>Session 2 - Room C</b> <i>Chair Catherine BELLE</i>	<b>Session 3 - Room D</b> <i>Chair Ewen BODIO</i>
11h10 - 11h40	<b>KN2 EINSLE Oliver</b> <i>Towards a Unified Concept of Nitrogenase Catalysis</i>	<b>KN4 TUCZEK Felix</b> <i>Model systems of copper-containing monooxygenases with pyridazine backbone</i>	<b>KN6 DAUMANN Lena</b> <i>Inspired by Nature: Separation of Lanthanides and Actinides</i>
11h40 - 12h00	<b>OC3 BERTEAU Olivier</b> <i>Crystallographic snapshots of Mmp10, a B12-dependent radical SAM methyltransferase involved in methane biosynthesis</i>	<b>OC7 STOKOWA Kamila</b> <i>Cu(II) and Fe(II) binding, DNA cleavage and radicals production by outer-membrane protein fragments from <i>F. nucleatum</i></i>	<b>OC11 ELISEEVA Svetlana</b> <i>Tuning functional properties of lanthanide(III)-based metallacrowns</i>
12h00 - 12h20	<b>OC4 ASH Philip</b> <i>Unifying Mechanism in NiFe Hydrogenase Using Advanced Spectroscopic Techniques</i>	<b>OC8 NEUMANN Wilma</b> <i>Dithiopyrrolones are Chelators that Mediate the Redox Cycling of Copper</i>	<b>OC12 HAMON Nadège</b> <i>Design of specific regio-fuctionalized pycen-based Ln(III) complexes for two-photon excitation and application to imaging or theranostic</i>
12h20 - 14h00 <b>LUNCH</b>			
<b>Discussion around Gender in Science</b>			
<i>Room A - Chair Carole DUBOC &amp; Pascale DELANGLE</i>			
	<b>Session 1 - Room B</b> <i>Chair Abhishek DEY</i>	<b>Session 2 - Room C</b> <i>Chair Luca BERTINI</i>	<b>Session 3 - Room D</b> <i>Chair Bas DE BRUIN</i>
15h00 - 15h30	<b>KN7 AUKAULOO Ally</b> <i>Coupling photoredox with bioinspired molecular catalysts for O<sub>2</sub> and CO<sub>2</sub> activation</i>	<b>KN9 PETOUD Stéphane</b> <i>Metals for Biological and Medical Diagnostics: Dual-mode Nearinfrared Optical and Photoacoustic Imaging Agent based on Low Energy Absorbing Ytterbium Complex</i>	<b>KN11 GALLO Emma</b> <i>Synthesis of Biologically Relevant Heterocycles Mediated by Porphyrin-based Catalysts</i>
15h30 - 15h50	<b>OC13 ARTERO Vincent</b> <i>Proton relays in molecular electrocatalysis: specifications for efficiency and insights into their relevance for reversible behavior</i>	<b>OC15 IVANOVIC-BURMASOVIC Ivar</b> <i>Is Zn redox "innocent"? Redox modulation and signaling by Zn vs Fe and Mn</i>	<b>OC17 SRNEC Martin</b> <i>On the role of asynchronicity and frustration in C-H bond activation by metal-oxo complexes</i>
15h50 - 16h10	<b>OC14 LOURO Ricardo</b> <i>Exploring the molecular mechanisms of electron uptake by (photo)electro-autotrophic organisms</i>	<b>OC16 GAMBINO Dinorah</b> <i>Multi-functional organometallic compounds as prospective antitrypanosomal agents: new approaches</i>	<b>OC18 AVENIER Frédéric</b> <i>Bioinspired Iron Chemistry: i) Heterolytic O-O Bond Breaking Reaction and ii) Unprotected Nitrene Transfer Reactions</i>
16h10 - 16h40	<b>KN8 MINTEER Shelley</b> <i>Enzymatic and Microbial Bioelectrocatalysis for Electrosynthesis</i>	<b>KN10 VILAR Ramon</b> <i>Targeting and imaging DNA with metal complexes</i>	<b>KN12 MORGAN Grace</b> <i>Dioxygen Activation by Electronic Modulation of Redox and Spin State Choice in Mn and Co Chelate Complexes</i>
16h40 - 17h10 <b>Coffee Break</b>			
<b>PL2 - Jana ROITHOVA</b>			
<b>Bioinspired catalysis investigated by mass spectrometry</b>			
<i>Room A - Chair Pascale MALDIVI</i>			
18h00 - 19h30 <b>Poster Session</b> <i>Hall SUD</i>			

8h30 - 9h20			
<b>PL3 - Nick LE BRUN</b>			
<b>Adventures with iron-sulfur cluster-containing regulators: elucidation of sensing mechanisms</b>			
<i>Room A - Chair Sandrine OLLAGNIER</i>			
	<b>Session 1 - Room B</b>	<b>Session 2 - Room C</b>	<b>Session 3 - Room D</b>
	<i>Chair Sven STRIPP</i>	<i>Chair Christelle HUREAU</i>	<i>Chair Shelley MINTEER</i>
9:30 - 10:00	<b>KN13 AGAPIE Theodor</b>	<b>KN15 BLINDAUER Claudia</b>	<b>KN17 HELLWIG Petra</b>
	<i>Cluster Models of the Nitrogenase Active Site</i>	<i>How marine cyanobacteria deal with zinc in an ocean desert</i>	<i>Electrocatalytic and Spectroscopic Studies on Cytochrome bd Oxidase, a Highly Diverse Bacterial Defense Factor</i>
10:00 - 10:20	<b>OC19 ANXOLABEHHERE Elodie</b>	<b>OC23 JANCOSO Attila</b>	<b>OC27 FOLGOSA Filipe</b>
	<i>Electrochemical O<sub>2</sub> activation by Fe and Mn porphyrins. Towards electrocatalytic aerobic oxidations of organic substrates</i>	<i>On the metal site stabilizing role of the C-terminal CCHHRAG fragment of the metalloregulatory protein CueR</i>	<i>The conserved amino acid motif -GSSYN- is essential for the E. coli flavorubredoxin NO reductase its activity</i>
10:20 - 10h40	<b>OC20 MILET Anne</b>	<b>OC24 KIELB Patrycja</b>	<b>OC28 ZHANG Huijie</b>
	<i>Theoretical Mechanistical Study of CO<sub>2</sub> Reduction to CH<sub>4</sub> by a Bio-Inspired NiFe Hydrogenase Model on graphite.</i>	<i>Do Tyr/Trp redox pathways protect O<sub>2</sub>-reducing S. Coelicolor laccase from oxidative damage?</i>	<i>Development of Multi-heme Cytochromes-Carbon Dots Biohybrids for Solar Chemicals and Fuels Generation</i>
<b>10h40-11h10 Coffee Break</b>			
	<b>Session 1 - Room B</b>	<b>Session 2 - Room C</b>	<b>Session 3 - Room D</b>
	<i>Chair Oliver EINSLE</i>	<i>Chair Jens MÜLLER</i>	<i>Chair Liviu MIRICA</i>
11h10 - 11h40	<b>KN14 HÖGBOM Martin</b>	<b>KN16 HANNON Mike</b>	<b>KN18 HERRES-PAWLIS Sonja</b>
	<i>Toward geometric structures of oxidized cofactors and high-valent metal-oxygen intermediates in di-metal proteins by femtosecond XFEL crystallography</i>	<i>Supramolecular recognition of DNA and RNA junction structures for anti-viral and anti-cancer therapy</i>	 <i>Manipulating the Electron Transfer in Entatic State Model - The Influence of Substituents on Novel Copper Guanidine Quinoline Complexes</i>
11h40 - 12h00	<b>OC21 WORRALL Jonathan</b>	<b>OC25 SIGEL Roland</b>	<b>OC29 KULAK Nora</b>
	<i>Serial femtosecond X-ray crystallography reveals the role of water molecules in the chemistry of compound I reduction in dye-decolorizing peroxidases</i>	<i>Programmed cell death and SARS-CoV-2; two RNA G-quadruplexes in the focus of metal ions, their complexes, and small molecules</i>	<i>Prodiginin derivatives and their Cu(II)-dependent antimicrobial and photoinduced anticancer activity</i>
12h00 - 12h20	<b>OC22 RABE Patrick</b>	<b>OC26 PRATIK Shah</b>	<b>OC30 RONCONI Luca</b>
	<i>X-ray free electron laser studies reveal dioxygen binding to isopenicillin N synthase induces correlated motions during catalysis</i>	<i>Noncanonical Head-to-Head Hairpin DNA Dimerization at Interfacial Binding Sites by Orange Emissive Silver Nanocluster</i>	<i>Tale of a successful failure: gold(III)-glycoconjugates as antiviral agents against SARS-CoV-2</i>
<b>12h20 - 14h00 LUNCH</b>			
<b>14h00 - 15h00 Discussion around Integrity in Science</b>			
<i>Room A - Chairs Sandrine OLLAGNIER &amp; Stéphane MENAGE</i>			
	<b>Session 1 - Room B</b>	<b>Session 2 - Room C</b>	<b>Session 3 - Room D</b>
	<i>Chair Pascale DELANGLE</i>	<i>Chair Vincent FOURMOND</i>	<i>Chair Jean-Pierre MAHY</i>
15h00 - 15h30	<b>KN19 HUREAU Christelle</b>	<b>KN21 NICOLET Yvain</b>	<b>KN23 PECORARO Vincent</b>
	<i>Natural polyanions to tune the metal-modulated self-assembly of Aβ amyloid-forming peptides</i>	<i>FeFe-hydrogenase active site assembly: the case of HydE</i>	<i>de Novo Designed Protein Catalysis</i>
15h30 - 15h50	<b>OC31 MIRICA Liviu</b>	<b>OC33 CASERTA Giorgio</b>	<b>OC35 CHAKRABORTY Saumen</b>
	<i>Novel Theranostic Agents for Alzheimer's Disease</i>	<i>Stepwise assembly of the [NiFe]-hydrogenase active site</i>	<i>De Novo Designed Artificial Cu Proteins (ArCuPs) as O-H/O-O/C-H Activation Catalysts</i>
15h50 - 16h10	<b>OC32 BERTINI Luca</b>	<b>OC34 STRIPP Sven</b>	<b>OC36 LEONE Linda</b>
	<i>Membrane damages induced by Cu(II)-Aβ•OH radical species. OH propagation toward polar head groups and lipid tails of membrane phospholipid</i>	<i>Proton-coupled Electron Transfer in the Catalytic Mechanism of [FeFe]-Hydrogenase</i>	<i>Unveiling selectivity in indole oxidation catalyzed by artificial heme-enzymes</i>
16h10 - 16h40	<b>KN20 GOSH DEY Somdatta</b>	<b>KN22 LEIMKÜHLER Silke</b>	<b>KN24 WARD Thomas</b>
	<i>Heme and Copper bound Amyloid β Peptides: Reactive Intermediates relevant to Oxidative Degradation of Neurotransmitters</i>	<i>Modulation of the Molybdenum Coordination Sphere of E. coli Trimethylamine N-oxide reductase and role of the nucleotides in the bis-MGD molybdenum cofactor</i>	<i>Artificial Metalloenzyme for in vivo Catalysis: Challenges and Opportunities</i>
<b>16h40 - 17h10 Coffee Break</b>			
<b>17h10 - 18h00 PL4 - Clotilde POLICAR</b>			
<b>Metal complexes in biological environments: a new frontier in inorganic chemistry</b>			
<i>Room A - Chair Vincent PECORARO</i>			
			
18h00 - 19h30	<b>Poster Session</b> <i>Hall SUD</i>		

<b>PL5 - Franc MEYER</b> <b>Unusual Spin States and Spin-Dependent Reaction Trajectories in Biorelevant Dicopper/O<sub>2</sub> and Diiron/NO Chemistry</b> <i>Room A - Chair Carole DUBOC</i>			
	<b>Session 1 - Room B</b> <i>Chair Fabrice THOMAS</i>	<b>Session 2 - Room C</b> <i>Chair Claudia BLINDAUER</i>	<b>Session 3 - Room D</b> <i>Chair Mike HANNON</i>
8h30 - 9h20			
9:30 - 10:00	<b>KN25 COMPANY Anna</b> <i>Exploring the oxidation chemistry of iron(V)-oxo-carboxylato species</i>	<b>KN27 FREISINGER Eva</b> <i>Metallothioneins – looking beyond the fully metalated state</i>	<b>KN29 MEZLER-NOLTE Nils</b> <i>New Chemistry of Organometallic Rhenium Complexes for Drug Development</i>
10:00 - 10:20	<b>OC37 ARRIGONI Federica</b> <i>Exploring novel features of [FeFe]-hydrogenase models through non-biomimetic modifications and reactivity: a DFT viewpoint</i>	<b>OC41 BYRNE Joseph</b> <i>Carbohydrate-functionalised metal complexes: targeting bacterial carbohydrate-binding proteins for therapeutic and sensing applications</i>	<b>OC45 COVERDALE James</b> <i>Advances in Os(II)-catalysed intracellular asymmetric reduction: new targets, stability improvement and anticancer potency enhancement</i>
10:20 - 10h40	<b>OC38 MARTINI Maria Alessandra</b> <i>Inhibition by CN<sup>-</sup> provides insight into the catalytic mechanism of [FeFe] hydrogenases</i>	<b>OC42 CORREIA Isabel</b> <i>Liposomal formulation of a new Zn(II) complex exhibiting high therapeutic potential in a murine colon cancer model</i>	<b>OC46 MASSAI Lara</b> <i>Internalization of Anticancer Gold(I) Complexes in Human H Ferritin to Improve Drug Selectivity</i>
10h40-11h10			
	<b>Session 1 - Room B</b> <i>Chair Emma GALLO</i>	<b>Session 2 - Room C</b> <i>Chair Ragnar BJORNSSON</i>	<b>Session 3 - Room D</b> <i>Chair Roland SIGEL</i>
11h10 - 11h40	<b>KN26 DE BRUIN Bas</b> <i>Bio-Inspired Synthesis of Ring Compounds using Metalloradical Catalysis</i>	<b>KN28 PEREIRA Ines</b> <i>High activity metalloenzymes for sustainable production of fuels</i>	<b>OC47 MÜLLER Jens</b> <i>Light-Induced Formation of Metal-Mediated Base Pairs</i>
11h40 - 12h00	<b>OC39 ZLATAR Matija</b> <i>Coordination preferences of Schiff base ligands with transition metals: DFT study</i>	<b>OC43 BIRRELL James</b> <i>Structural insights on the mechanism of the electron-bifurcating [FeFe] hydrogenase from <i>Thermotoga maritima</i></i>	<b>OC48 SANTOS Joana</b> <i>Mitochondria-targeted Radiocomplexes for Auger Electron Therapy of Cancer</i>
12h00 - 12h20	<b>OC40 SILAGHI-DUMITRESCU Radu</b> <i>Old dogs, old tricks, new glasses: hydrogen peroxide, cobalamin and others</i>	<b>OC44 FOURMOND Vincent</b> <i>Exploring the reactivity of CO dehydrogenases</i>	<b>OC49 VAZQUEZ LOPEZ Miguel</b> <i>Selective Cleavage of DNA Replication Foci in Cell Nuclei by Peptide Helicates</i>
<b>FREE AFTERNOON - ACTIVITIES AROUND GRENOBLE</b>			
19h30	<b>GALA DINER</b> <b>Stade des Alpes</b> Boulevard Jean Pain 38000 Grenoble Tram station "Grenoble Hôtel de Ville"		

8h30 - 9h20			
<b>PL6 - Gerard ROELFES</b>			
<b>Artificial Metalloenzymes going Live</b>			
<i>Room A - Chair Thomas WARD</i>			
	<b>Session 1 - Room B</b>	<b>Session 2 - Room C</b>	<b>Session 3 - Room D</b>
	<i>Chair Luca RONCONI</i>	<i>Chair Dinorah GAMBINO</i>	<i>Chair Philip ASH</i>
9:30 - 10:00	<b>KN30 PIKRAMENOU Zoe</b> <i>Luminescent Nanoparticles in detection and triggered drug release</i>	<b>KN32 SUMAN Sigridur</b> <i>Molybdenum Complexes as Catalytic Cyanide Antagonists: Biocompatibility, Intracellular Distribution and Mechanism.</i>	<b>KN35 LEPOUL Nicolas</b> <i>Electrochemical and spectroelectrochemical approaches for the characterization of transient copper-oxygen models of oxygenases</i>
10:00 - 10:20	<b>OC50 BODIO Ewen</b> <i>Aza-BODIPY and metal, a winning association for multimodal imaging and theranostics</i>	<b>OC55 PIZZARO Ana</b> <i>Potent Tethered Osmium(III) Half-Sandwich Anticancer Agents Bearing Phenylpyridine</i>	<b>OC59 GUIGLIARELLI Bruno</b> <i>Deciphering the Metal Ion Environment in Formate Dehydrogenases: Insights from EPR, Isotopic Enrichment and DFT Calculations in a Tungsten and Selenium Dependent Enzyme</i>
10:20 - 10h40	<b>OC51 MOLLOY Jennifer</b> <i>Design and synthesis of a multitopic pro radical probe for the detection of oxidative stress</i>	<b>OC56 ENYEDY Eva</b> <i>Water-soluble 8-hydroxyquinoline-amino acid hybrids and their interaction with various metal ions: relationship between solution chemistry and cytotoxicity</i>	<b>OC60 GHATTAS Wadiah</b> <i>Artificial metalloenzymes for in vitro and in vivo catalysis</i>
10h40-11h10 <b>Coffee Break</b>			
	<b>Session 1 - Room B</b>	<b>Session 2 - Room C</b>	<b>Session 3 - Room D</b>
	<i>Chair Olivier BERTEAU</i>	<i>Chair Attila JANCSCO</i>	<i>Chair Frédéric AVENIER</i>
11h10 - 11h40	<b>KN31 CIOFI BAFFONI Simone</b> <i>The intriguing puzzle of iron-sulfur protein biogenesis</i>	<b>KN33 GUMIENNA-KONTECKA Elzbieta</b> <i>Inspired by siderophores: from structural probes of ferric ions assimilation to Ga-68/Zr-89 nuclear imaging</i>	<b>KN36 SHOJI Osami</b> <i>Hydroxylation of Nonnative Substrates by Wild-type Cytochrome P450BM3 with Decoy Molecules</i>
11h40 - 12h00	<b>OC52 MOUGEL Victor</b> <i>Iron-sulfur clusters: synthetic challenges and applications to catalysis</i>	<b>OC57 MICHAUD-SORET Isabelle</b> <i>Is the iron homeostasis under the control of an iron-sulfur cluster in Fur?</i>	<b>OC61 HAGEDOORN Peter-Leon</b> <i>Unique Biradical Intermediate in the Mechanism of the Heme Enzyme Chlorite Dismutase discovered using microsecond timescale freeze hyperquench</i>
12h00 - 12h20	<b>OC53 CUTSAIL George</b> <i>Stabilization of Intermediate Spin-States in Mixed-valent Diiron Dichalcogenide Complexes</i>	<b>OC58 RODRIGUEZ MACIA Patricia</b> <i>How accessory iron-sulfur clusters influence catalytic bias, O2 tolerance and overpotential in [FeFe] hydrogenases</i>	<b>OC62 GYURCSIK Béla</b> <i>Interplay of multiple metal ion binding sites regulates the catalytic activity of metalloenzymes</i>
12h20 - 12h50	<b>OC54 DECAMPS Laure</b> <i>Nitrogenase P-cluster biosynthesis: unraveling the role of NifW with spectroscopy</i>	<b>KN34 SCHALK Isabelle</b> Cancelled	<b>KN37 TRON Thierry</b> <i>Hybrid catalysis and Multi-Copper oxidases</i>
12h50 - 14h30 <b>LUNCH</b>			
<i>Room A - Chair Stéphane MENAGE</i>			
14h30 - 15h20	<b>PL7 Marc FONTECAVE</b> <i>From CO<sub>2</sub> to fuels: bioinspired metal catalysts</i>		
15h20 - 15h50	<i>Room A - Chair Eva FREISINGER</i> <b>EUROBIC Medal 2022 - Maxie ROESSLER</b> <i>Controlling and exploiting intrinsic unpaired electrons in metalloproteins</i>		
15h50 - 16h20	<b>Closing Ceremony - Eurobic Awards</b> Chairs : Carole DUBOC - Stéphane MENAGE		
16h20 - 17h00	Coffee Break		