

## PROGRAMME JED 2016

8h00-9h00	Accueil des participants, installation des posters		
9h00-9h30	<b>Présentation d'Introduction à la JED</b> par Christophe Colbeau-Justin, <b>Amphi Jules Horowitz</b>		
9h30-10h15	<b>Conférence plénière</b> , Gilberte Chambaud, Présidente de la SCF, <b>Amphi Jules Horowitz</b> <i>From Alchemy to computational chemistry: concept of chemical bond.</i>		
10h15-11h00	Pause café / posters, Salles A8+A10-Bat 399		
<b>Communications orales</b>			
Pôle CPBA, Amphi Jules Horowitz	Pôle COB, Salle B6 – Bat 399	Pôle CIM, Salle 112 – Bat 395	
Modérateur : Eric Eliot	Modérateur : Corinne Gosmini	Modérateur : Pierre Mialane	
11h00-11h15	Pierre Barbier Saint-Hilaire	Djamil Azazna	Lucile Fétiveau
11h15-11h30	Marta Bolsa Ferruz	Remy Campagne	Rana Choumane
11h30-11h45	Luisa Carvalho	Maxime Giardinetti	Amandine Boulmier
11h45-12h00	Mbaye Faye	Valentin Magné	Alicia Aloisi
12h00-12h15	Seif Bennia	Hajar Mamad-Hemouch	Manuel Antuch-Cubillas
12h15-14h00	Pause déjeuner / posters, Salles A8+A10-Bat 399		
<b>Conférences invitées</b>			
Pôle CPBA, Amphi Jules Horowitz	Pôle COB, Salle B6 – Bat 399 Rdc	Pôle CIM, 112 – Bat 395	
Hubert Girault	Laurence Grimaud	Guillaume Rogez	
<i>From grid to mobility: Megabatteries &amp; on-site hydrogen production</i>		<i>Mechanistic Studies for more rationale developments of new methodologies</i>	
Modératrice : Marie-Pierre Gaigeot		<i>Fonctionnalisation d'hydroxydes et d'oxydes lamellaires : insertion, greffage, réaction in situ... et micro-ondes</i>	
Modératrice : Marie-Pierre Gaigeot		Modérateur : Sébastien Floquet	
<b>Communications orales</b>			
14h30-14h45	Dita Floresyona	Joëlle Char	Mathieu Xémard
14h45-15h00	Ludmilla Guduff	Ahmad Kassir	Benjamin Cahier
15h00-15h15	Elisabetta Pancani	Anne-Sophie Marques	Benjamin Hary
15h15-15h30	Emmanuel Jaccoulet	Anaëlle Doerflinger	Mhamad Aly Moussawi
15h30-15h45	Madanakrishna Katari	Clément Lepori	Fabien Nassoy
15h45-16h30	Pause café / posters, Salles A8+A10-Bat 399		
<b>Communications orales</b>			
Pôle CPBA, Amphi Jules Horowitz	Pôle COB, Salle B6 – Bat 399 Rdc	Pôle CIM, 112 – Bat 395	
Modératrice : Hynd Remita	Modérateur : Arnaud Voituriez	Modérateur : Sophie Peulon	
16h30-16h45	Xue Li	Longhui Gao	Tawfiq Nasr Allah
16h45-17h00	Allan Lopes	Pierre Quinodoz	Kevin Dedecker
17h00-17h15	Jérôme Mahé	Marie Vayer	Dalila Bounoua
17h15-17h30	Ariel-Francis Perez-Mellor	Yang Wan	Clémence Ducloiset
17h30-17h45	Anja Roeder	Nacim Zidelmal	Irène Mustieles-Marin
18h00-18h30	Clôture, remise des prix, Amphi Jules Horowitz		

**Communications orales CPBA**

Pierre Barbier Saint-Hilaire : **Metabolomics of CerebroSpinal Fluid and Plasma for the Caracterisation of Hepatic Encephalopathy.** SPI, CEA, Université Paris-Sud.

Marta Bolsa Ferruz : **New insights into metallic nanoparticles for enhancement of particle therapy in hypoxic tumors.** ISMO, CNRS, Université Paris-Sud.

Luisa Carvalho : **Growth of micrometric oxide layers for the study of metallic surfaces decontamination by laser.** SEARS, CEA, Université Paris-Sud.

Mbaye Faye : **On the use of difference bands for modeling SF6 absorption in the 10µm atmospheric window.** SOLEIL, Université Paris-Sud.

Seif Bennia : **Characterization Of Fulleropyrrolidine by HR-MS and NMR Spectroscopy.** ICMMO, CNRS, Université Paris-Sud – LMMA, IPEST, Tunisie.

Dita Floresyona : **Metal and Polymer Nanostructures Synthesized in Swollen Hexagonal Mesophases: Application in Fuel Cells.** LCP, CNRS, Université Paris-Sud.

Ludmilla Guduff : **Fast multidimensional diffusion-based NMR analysis of mixtures.** ICSN, CNRS, Université Paris-Sud.

Elisabetta Pancani : **Development, characterization and pulmonary administration of biodegradable nanoparticles encapsulating a synergic drugs combination to treat tuberculosis.** ISMO, CNRS, Université Paris-Sud.

Emmanuel Jaccoulet : **Identification of Therapeutic Monoclonal Antibodies by Capillary Electrophoresis or Flow Injection Spectroscopy coupled to Multivariate Analysis.** Institut Galien, CNRS, Université Paris-Sud.

Madanakrishna Katari : **Electronic structure of reduced organometallic complexes in gas phase.** LCM, CNRS, Ecole Polytechnique.

Xue Li : **Design of Metal-Organic Frameworks nano- and micro- particles as efficient drug carriers.** ISMO, CNRS, Université Paris-Sud.

Allan Lopes : **Gas-Phase Ion-Molecule Chemistry : An experimental study of the reaction of CH<sub>3</sub><sup>+</sup> with CH<sub>4</sub> and other hydrocarbons.** LCP, CNRS, Université Paris-Sud.

Jérôme Mahé : **Far-IR spectroscopy of neutral gas phase peptides: signatures from combined experiments and simulations.** LAMBE, Université d'Evry Val d'Essonne.

Ariel-Francis Perez-Mellor : **Bi-Chromophoric chiral peptides studied by conformation-sensitive vibrational spectroscopy.** ISMO, CNRS, Université Paris-Sud.

Anja Roeder : **Femtosecond dynamics of the 2-methylallyl radical in the gas phase.** LIDyL, CEA, Université Paris-Sud.

## Communications orales COB

Djamil Azazna : **Study of a new family of Bambus[n]urils.** SCBM, CEA, Université Paris-Sud.

Remy Campagne : **New Strategies for Alkaloid Synthesis: Nitroso Diels-Alder and C-H Insertion Reactions.** ICMMO, CNRS, Université Paris-Sud.

Maxime Giardinetti : **Synthesis and fluorescence studies of tricyclic indole derivatives.** ILV, Université de Versailles Saint-Quentin.

Valentin Magné : **Synthesis of spiro[piperidine-3,3'-oxindoles] via gold(i)-catalysed dearomatization of n-propargyl-2-bromotryptamines.** ICSN, CNRS, Université Paris-Sud.

Hajar Mamad-Hemouch : **Synthesis of cyclodextrin nanotubes based on a polyrotaxane.** LAMBE, Université d'Evry Val d'Essonne.

Joëlle Char : **Synthesis of Aromatic Sulfones from SO<sub>2</sub> and Organosilanes, Under Metal-free Conditions.** NIMBE, CEA, Université Paris-Sud.

Ahmad Kassir : **Synthesis of all four stereoisomers of oxetin by a photochemical approach.** ICMMO, CNRS, Université Paris-Sud.

Anne-Sophie Marques : **Iron-mediated dearomative (3+2) cycloaddition between oxyallyl cations and N-acetyl indoles.** ILV, Université de Versailles Saint-Quentin.

Anaëlle Doerflinger : **Design and synthesis of polymerized micelles for the diagnosis and therapy of tumors.** SCBM, CEA, Université Paris-Sud.

Clément Lepori : **Low-valence iron and cobalt complexes: difference of reactivity in hydroamination of alkenes.** ICMMO, CNRS, Université Paris-Sud.

Longhui Gao : **Deuterium labelling of thioether substructures in bioactive molecules.** SCBM, CEA, Université Paris-Sud.

Pierre Quinodoz : **From 2-cyanoazetidines to multi-click reactions: an eventful journey.** ILV, Université de Versailles Saint-Quentin.

Marie Vayer : **Acid-catalysed intramolecular addition of β-ketoesters to 1,3-dienes.** ICMMO, CNRS, Université Paris-Sud.

Yang Wan : **Synthesis of Original γ-Amino Acids and Their Use to Build New Peptide Structures.** ICMMO, CNRS, Université Paris-Sud.

Nacim Zidemal : **Synthesis of chiral salen-based monomers for silica supported controlled polymerization-new materials for asymmetric heterogeneous catalysis.** ICMMO, CNRS, Université Paris-Sud.

## Communications orales CIM

Lucile Fétiveau : **Contrast agents based on Prussian blue analogues.** *ICMMO, CNRS, Université Paris-Sud.*

Rana Choumane : **Studies of the reactivity of manganese compounds versus heavy metals : Applications for the development of innovative decontamination devices.** *LAMBE, Université d'Evry Val d'Essonne.*

Amandine Boulmier : **Polyoxometalate Bisphosphonate Complexes: Synthesis, Structure and Activity on Tumor Cell Lines.** *ILV, Université de Versailles Saint-Quentin.*

Alicia Aloisi : **Complexes of tripodal phosphine ligands: synthesis, structure and catalytic activity in the hydroboration of CO<sub>2</sub>.** *NIMBE, CEA, Université Paris-Sud.*

Manuel Antuch-Cubillas : **Catalytic tuning of Rh doped SrTiO<sub>3</sub> photoelectrodes with Co clathrochelates for water splitting.** *ICMMO, CNRS, Université Paris-Sud.*

Mathieu Xémard : **Highly reactive divalent lanthanide precursors and polymetallic species.** *LCM, Ecole Polytechnique.*

Benjamin Cahier : **Symmetry in spin-orbit coupling and magnetic anisotropy in mononuclear transition metal complexes.** *ICMMO, CNRS, Université Paris-Sud.*

Benjamin Hary : **Influence of the nano-precipitates content and cold-working on the recrystallization in ferritic ODS steels.** *CEA - ICMMO, CNRS, Université Paris-Sud.*

Mhamad Aly Moussawi : **Supramolecular organic/inorganic assemblies.** *ILV, Université de Versailles Saint-Quentin.*

Fabien Nassoy : **Vertically aligned carbon nanotubes growth on aluminium substrates at low temperature.** *NIMBE, CEA, Université Paris-Sud.*

Tawfiq Nasr Allah : **Unprecedented iron catalysts for the carbonylation of amines.** *NIMBE, CEA, Université Paris-Sud.*

Kevin Dedecker : **Design of multifunctional hybrid materials for capture of Volatile Organic Compounds (VOCs): Application to cultural heritage preservation.** *ILV, Université de Versailles Saint-Quentin.*

Dalila Bounoua : **Single crystal growth and physical properties of the pristine and doped one-dimensional spin chains cuprate SrCuO<sub>2</sub> and Sr<sub>2</sub>CuO<sub>3</sub>.** *ICMMO, CNRS, Université Paris-Sud.*

Clémence Ducloiset : **Studies of di-rhodium complexes for reactions by Nitrogen Atom Transfer.** *ICMMO, CNRS, Université Paris-Sud.*

Irène Mustieles-Marin : **One-electron oxidation of copper and nickel phosphasalen complexes.** *LCM, Ecole Polytechnique.*

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