

**1<sup>st</sup> Women in Supramolecular Chemistry (WISC) workshop: an introduction to Supramolecular Chemistry techniques for early stage career researchers**

**6th-8th September 2021**

**PROGRAMME**

**Monday, September 6<sup>th</sup>, 2021**

**8h30** Registration

**9h15** Opening Ceremony

*Chair Prof Vito Lippolis (University of Cagliari)*

**09h30** PL1 **Prof Ivan Huc** (Ludwig Maximilians University)

*“Aromatic foldamers: engineering molecular shape”*

**10h20** OC1 **Christel Dolain** (University of Bordeaux)

*“Towards the Design and Synthesis of Multi-Stranded  $\beta$ -Sheet Foldamers”*

**10h35** OC2 **Maria Magdalena Cid** (Universidade de Vigo)

*“Molecular Recognition Phenomena detected by Helicoidal Signals”*

**10h50** OC3 **Morgane Pasco** (University of Bordeaux)

*“De Novo design and synthesis of artificial helical barrels: toward enzyme mimics”*

**11h05** Coffee break

Chair Prof Kay Severin (Ecole Polytechnique Fédérale de Lausanne)

**11h25** IL1 **Prof Valeria Amendola** (University of Pavia)

*“Azacryptands: versatile molecular cages for recognition and separation processes”*

**11h55** OC4 **Mindy Levine** (Ariel University)

*“Cyclodextrin Complexation: Flexible Molecules with Surprising Chemical Insights”*

**12h10** OC5 **Neha Rani Kumar** (Dhemaji College)

*“Thienyltriazine Based Porous Polymers of Tunable Properties”*

**12h25** OC6 **Anna Wcisło** (University of Gdańsk)

*“Self-assembling layers on the surface of conductive materials - properties and applications”*

**12h40** OC7 **Valentina Corvaglia** (Ludwig Maximilians University)

*“DNA mimic foldamers: structural features and biological applications”*

**12h55** OC8 **Eleonora Macedi** (University of Urbino)

*“A  $\text{Cu}^{2+}/\text{Ca}^{2+}/\text{Ca}^{2+}/\text{Cu}^{2+}$  platform for anion binding and sensing”*

**13h10** **Lunch break**

*Chair Prof Valérie Heitz (Université de Strasbourg)*

**14h30** PL2 **Prof Michael J. Hardie** (University of Leeds)

*“Crystallographic characterisation of large metallo-supramolecular assemblies”*

**15h20** OC9 **Riccardo Montis** (University of Urbino)

*“Complex structures for a simple organic salt: the extraordinary self-assembly of Fampridine Hydrochloride”*

**15h35** OC10 **Iris Solymosi** (Friedrich-Alexander-University Erlangen-Nuremberg)

*“Perylene bisimide cyclophane-fullerene hybrids with homochiral recognition”*

**15h50** OC11 **Claire Fave** (Université de Paris)

*“Synergy between electrochemistry and sigma-hole interactions: from anion recognition to catalysis”*

**16h05** **Coffee break**

*Chair Prof Luisa De Cola (University of Milano)*

**16h25** IL2 **Prof Luca Prodi** (University of Bologna)

*“Dye doped silica nanoparticles as photoactive organized systems for nanomedicine”*

**16h55** OC12 **Ariadna Lazaro** (Universitat de Barcelona)

*“Promoting excimer formation in [N<sup>+</sup>C<sup>-</sup>N] cyclometallated platinum(II) compounds with aromatic alkynyl ligands”*

**17h10** OC13 **Gustavo A. Zelada-Guillén** (National Autonomous University of Mexico)

*“Tuning supramolecular response in polymer-graphene hybrid nanomaterials for novel flexible portable sensors”*

**17h25** OC14 **Sameh El Sayed** (University of Birmingham)

*“Selective and sensitive detection of cyanide and sulfide in water by metal-macrocycle-based capped silica mesoporous nanoparticles”*

**17h40** OC15 **Carina I. C. Crucho** (Universidade de Lisboa)

*“Smart polystyrene-silica core-shell nanoparticles”*

**17h55** IL3 **Prof Laura Rodriguez** (Universitat de Barcelona)

*“Supramolecular assemblies and luminescence of gold and platinum organometallic complexes”*

**18h25** Poster session (3 min presentation)

*Chair Dr Giacomo Picci (University of Cagliari)*

B1 **Dana Kauerhof** (University of Duisburg-Essen)

*“Heterobifunctional catenanes and rotaxanes for cooperative organocatalysis”*

B2 **Maike Thiele** (University of Duisburg-Essen)

*“Complementary double helix formation through hydrogen-bond formation of chiral BINOL-derivatives”*

**B3 Zongyao Zhang** (University of Oxford)

*“Halogen bonding strapped porphyrin BODIPY rotaxanes for dual optical and electrochemical anion sensing”*

**B4 Araceli de Aquino** (Universitat de Barcelona)

*“Promoting the heavy atom effect on luminescent supramolecular Au(I) complexes”*

**B5 Tobias Paschelke** (Christian-Albrechts-Universität zu Kiel)

*“Copper-Free One-Pot Sonogashira-Type Coupling for the Efficient Preparation of Symmetric Diarylalkyne Ligands for Metal-Organic Cages”*

**B6 Guillermo Romo Islas** (Universitat de Barcelona)

*“Aggregation-induced emission enhancement in bimetallic Pt(II) pincers”*

**B7 Luca Conti** (University of Florence)

*“Highly charged ruthenium(II) polypyridyl complexes for the development of potential PDT agents”*

**B8 David Magri** (University of Malta)

*“Applications of Pourbaix Sensors: Molecular Logic Gates for Acidity and Oxidisability”*

**B9 Anurag Singh** (Université libre de Bruxelles)

*“Calixarenes with halogen bond donors for anion transport”*

**B10 Amrutha Prabodh** (Karlsruhe Institute of Technology)

*“Fluorescence Detected Circular Dichroism (FDCCD) for supramolecular host-guest complexes”*

**B11 Selina Hollstein** (University of Ulm)

*“Self-assembly of anion receptors based on orthoesters”*

**B12 Marianne Engeser** (University of Bonn)

*“Gas-phase fragmentation of metallo-supramolecular aggregates”*

**B13 Melina Knezevic** (University of Basel)

*“Tweezer directed C-H Oxidation”*

**B14 Daria Sokolova** (University of Basel)

*“Optimized iminium-catalysed 1,4-reductions inside the resorcinarene capsule: Achieving >90% ee with proline as catalyst”*

**B15 Patrizia Jankovic** (University of Rijeka)

*“Design of short catalytic sequences inspired by enzymatic active sites”*

**B16 Andrea Pinto** (Universitat de Barcelona)

*“Near unity fluorescent quantum yields of gold(I) benzothiadiazole-based derivatives in organic matrixes”*

**B18 Alexandra Heidecker** (Technical University Munich)

*“Analyzing hexacationic Ag(I)-Pillarplex dodecylammonium pseudorotaxane towards Location and Influence of Interaction Sites in the Solid-State Structure”*

**B19 Lau Halgreen** ((Université libre de Bruxelles)

*“Dynamic combinatorial chemistry with imines for the development of phosphate receptors”*

**B20 Thomas Pickl** (Technical University Munich)

*“Expanding the scope of macrocyclic poly-NHC ligands: bimetallic palladium(II) and platinum(II) complexes”*

**B21 Aaron Torres-Huerta** (Université libre de Bruxelles)

*“Transport of Carboxylates across lipid bilayer membranes”*

**B22 Gina Elena Giacomazzo** (University of Florence)

*“Nitroimidazole-based ruthenium(II) complexes: playing with structural parameters to design photostable and light-responsive antibacterial agents”*

**B23 Rui Kang** (Karlsruhe Institute of Technology)

*“Self-Assembly Probes (SAPs) solve the selectivity problem of the artificial chemosensors”*

B25 **João Carlos Lima** (Universidade Nova de Lisboa)

*“Gold(I)-doped films as efficient room temperature phosphorescent materials”*

**Tuesday, September 7<sup>th</sup>, 2021**

*Chair Prof. Claudia Caltagirone (University of Cagliari)*

**09h00** PL3 **Prof Jonathan W. Steed** (Durham University)

*“Supramolecular Gels and how to think about them”*

**09h50** WISC Event

**11h00 Coffee break**

*Chair Prof Laura Rodriguez (Universitat de Barcelona)*

**11h20** IL4 **Prof Hennie Valkenier** (Université libre de Bruxelles)

*“Monitoring transmembrane transport of ions using fluorescence spectroscopy”*

**11h50** OC16 **Laura Bickerton** (University of Oxford)

*“Highly active halogen bonding and chalcogen bonding chloride transporters with non-protonophoric activity”*

**12h05** OC17 **Rebecca Randle** (University of Glasgow)

*“Effect of pH and functionalisation of self-assembled naphthalene diimides for smart window applications”*

**12h20** OC18 **Rashmi Sharma** (IISER Pune)

*“Transmembrane anion- selective ion channels by self-assembled bis(cholate) derivatives”*

**12h35** OC19 **Alessio Cataldo** (Université libre de Bruxelles)

*“Direct monitoring of transmembrane transport of fluoride via fluorometric method”*

**12h50** OC20 **Daniela Kalafatovic** (University of Rijeka)

*“Application of soft computing in peptide design”*

**13h05** Lunch break

**16h45-20h00** Cagliari walking tour and aperitif

**Wednesday, September 8<sup>th</sup>, 2021**

*Chair Prof Hennie Valkenier (Université libre de Bruxelles)*

**09h00** PL4 **Prof Valérie Heitz** (Université de Strasbourg)

*“Supramolecular switchable cages from design to functional systems with the help of various techniques to characterize the systems and solve problems”*

**09h50** OC21 **Barbara Scholz** (Friedrich-Alexander-Universität Erlangen-Nürnberg FAU)

*“Tetrabenzoporphyrin Tweezers for Supramolecular Interactions”*

**10h05** OC22 **Sonia La Cognata** (University of Pavia)

*“Azacryptands as fillers in Mixed Matrix Membranes for Gas Separation”*

**10h20** OC23 **Amy Edo-Osagie** (Université de Strasbourg)

*“Porphyrin-acridinium conjugates: Developing multi-responsive receptors”*

**10h35** IL5 **Prof Kay Severin** (Ecole Polytechnique Fédérale de Lausanne)

*“Construction and Destruction of Coordination Cages”*

**11h05 Coffee break**

Chair Prof Ivan Huc (Ludwig Maximilians University)

**11h20** IL6 **Prof Ross S. Forgan** (University of Glasgow)

*“Tuning properties and functionality in the modulated self-assembly of metal-organic frameworks”*

**11h50** OC24 **Simone I.S. Hendrikse** (The University of Melbourne)

*“Bioinspired preorganised peptide-nucleotide nanofibers”*

**12h05** OC25 **Valentyna Slyusarchuk** (Keele University)

*“Fecht’s acid revisited: a rigid non-aromatic building block for metallosupramolecular chemistry”*

**12h20** OC26 **Fatima Aparicio** (Universidad Autónoma de Madrid)

*“Water soluble nanotubular architectures from amphiphilic dinucleobases”*

**12h35** OC27 **Giada Mannias** (University of Cagliari)

*“pH effect on the mechanochemical synthesis of an iron(III) trimesate Metal Organic Framework”*

**12h50** OC28 **Isabel Abánades Lázaro** (Universidad de Valencia)

*“Defect engineering of Titanium MOFs for enhanced catalytical applications”*

**13h05** OC29 **Deborah Romito** (Cardiff University/University of Vienna)

*“Chalcogen bonding as supramolecular tool for self-assembled layers in optoelectronic devices”*

**13h20** **Lunch break**

*Chair Prof David Magri*

**14h30** PL5 **Prof Luisa De Cola** (University of Milano)

*“Seeing is believing: how and why to visualize self-assembly processes”*

**15h20** OC30 **Ingrid Suzana** (Sorbonne Université)

*“Functional hetero-poly-metallic complexes”*

**15h35** OC31 **Zoey Warmerdam** (University of Victoria)

*“Diversity-oriented supramolecular host-guest chemistry targeting drugs and metabolites”*

**15h50** OC32 **Jessica Groppi** (University of Bologna)

*“The evolution of light effected autonomous molecular pumps”*

**16h05** **Coffee break**

*Chair Dr Riccardo Montis (University of Urbino)*

**16h25** **Best Poster Presentation**

**16h45** OC33 **Tainah D. Marforio** (University of Bologna)

*“Exploiting supramolecular protein chemistry to design biocompatible host-carriers for carboranes in BNCT”*

**17h00** OC34 **Allison Selinger** (University of Victoria)

*“Drugs that bind other drugs: template synthesis of bivalent reversal agents”*

- 17h15**      OC35 **Witri Wahyu Lestari** (Sebelas Maret University)  
*“Mixed Matrix Membrane based on Poly(ether-Sulfone) and MOF type of MIL-53(Al): Synthesis and Application in CO2 Gas Separation”*
- 17h30**      OC36 **Giulia Monceli and Marta DaPian** (Elsevier B.V.)  
*“Synthesis of responsive tetra-urea calix[4]arenes and calix[4]pyrroles: a combined experimental and predictive chemical approach”*
- 17h45**      Closing ceremony