

## Monday

### Physical Foundations of Organic Reactivity

#### Session 1a

- IL1 - **Henrik Ottosson**, Relating the Triplet State Baird-Aromaticity of the Macrocycle to that of the Monocycle
- O1 - **Yoshimitsu Itoh**, Ring Inversion Kinetics of Photoexcited Chiral [4n]Annulene Derivatives: Energetic Impact of Baird Aromaticity
- O2 - **Goetz Bucher**, Quenching of Triplet and Singlet Excited States by Carbon Dioxide
- O3 - **Gavin Jones**, Theoretical Studies on Ring-opening Polymerizations by Alkoxides and (Thio)ureas
- O4 - **Renana Gershoni-Poranne**, Aromatic Additivity in Three Dimensions

Coffee Break

#### Session 1b

- O5 - **Anat Milo**, Physical Organic Principles for Controlling the Secondary Sphere in Organocatalysis
- O6 - **Charles Perrin**, Approach Control. Stereoelectronic Origin of Geometric Constraints on N-to-S and N-to-O Acyl Shifts in Peptides
- O7 - **Leonor Cruzeiro**, A Kinetic Pathway for Protein Folding in vivo
- O8 - **Artur Mardyukov**, Unravelling Lawesson's Reagent – The Structure of Monomeric (4-Methoxyphenyl)phosphine Disulfide
- O9 - **Kazuhide Nakata**, Computational Study of Substituent Effects on Gas-Phase Stabilities of Amino(phenylboranyl)methyl Anions

### Reaction mechanisms and Catalysis

#### Session 2a

- IL2 - **Herbert Mayr**, Nucleophilicity and Electrophilicity Parameters for the Analysis of Cycloaddition Reactions
- O10 - **Michael Page**, Kinetics and mechanisms of organo-iridium catalyzed reactions
- O11 - **Igor V. Alabugin**, Coupling N-H deprotonation, C-H activation and oxidation: metal-free C(sp<sup>3</sup>)-H aminations with unprotected anilines
- O12 - **Xin Li**, Modeling Structure-Stereoselectivity Relationship Using Steric and Electronic Parameters for Chiral Bifunctional Tertiary-amine Thioureas Catalysis
- O13 - **Eduardo Humeres**, Desulfurization route of carbons modified with SO<sub>2</sub>. Polymerization of the sulfur allotropes intermediates

Coffee Break

### Session 2b

- O14 - **Einar Uggerud**, C–C bond formation of Mg and Zn activated carbon dioxide
- O15 - **Daisuke Kaneno**, Regioselectivity and Reaction Mechanism on Tricyanovinylolation of Pyrrole Derivatives
- O16 - **Joaquim Faria**, Chemical Modification of g-C<sub>3</sub>N<sub>4</sub> by beta-Cyclodextrin for Enhanced H<sub>2</sub> Photocatalytic Generation
- O17 - **Alexey Ignatchenko**, Beta keto acids: structure, reactivity, and formation as elusive intermediates in heterogeneous catalysis
- O18 - **Niklaas J. Buurma**, Predicting Racemisation Risk to Avoid Pointless Stereoselective Syntheses

### Supramolecular and Systems Chemistry

#### Session 3a

- IL3 - **Shuichi Hiraoka**, Nanocube: Hyperthermostable Discrete Self-Assemblies in Water
- O19 - **Sota Sato**, Chiral Intertwined Spirals and Chiroptical Properties Dictated by Cylinder Helicity
- O20 - **Thierry Brotin**, Molecular Recognition of Cations by Enantiopure Cryptophanes
- O21 - **Hrvoj Vančik**, Reaction mechanisms in crystalline molecular solids and their general importance in physical organic chemistry: a case study
- O22 - **Tatiana Nekipelova**, Aggregation-induced Chemical Reaction: Annulation of Acetylenes with Mixed Phosphonium-Iodonium Ylides

Coffee Break

#### Session 3b

- O23 - **Philippe Lainé**, From single-electron processes to multielectron handling and storage at the molecular level: designing super-electrophores
- O24 - **Nuno Basilio**, Stimuli-Responsive Supramolecular Systems Based on Bio-Inspired Molecular Switches
- O25 - **Laura Salonen**, A Supramolecular Strategy to High-Quality Covalent Organic Frameworks
- O26 - **Samuel Guieu**, Organic fluorophores in confined environment: properties and applications
- O27 - **Ofer Reany**, Hetero-Bambusurils

## Tuesday

### Physical Foundations of Organic Reactivity

#### Session 1c

- IL4 - **Robert McMahon**, Astrochemistry: A Perspective from Physical-Organic Chemistry
- O28 - **Ian Williams**, Influence of Dielectric Environment upon Isotope Effects on Glycoside Heterolysis: Computational Evaluation and Atomic Hessian A
- O29 - **John Wallis**, New Studies of Interactions and Bond Formation in Peri-Naphthalenes
- O30 - **Jiří Váňa**, On the Way from Understanding of Basic Principles to Rational Design of Reaction Conditions for Palladium Catalysed C–H Activation
- O31 - **Luís Duarte**, Interaction of Formic Acid with Nitrous Oxide and Carbon Monoxide
- O32 - **Igor Reva**, Spontaneous and Photochemically Induced Reactions of Triplet 2-Formyl-Phenylnitrene in Low-Temperature Matrix

### SESSÃO 2 - Reaction mechanisms and Catalysis

#### Session 2c

- IL5 - **Halina Szatyłowicz**, Physical Interpretation of the Substituent Effect – the Quantum Chemistry Approach
- O33 - **Hendrik Zipse**, Size-Induced Chemoselectivity in Esterification Reactions
- O34 - **Victor Chechik**, A new approach to detect short-lived radicals: application to atmospherically-relevant radicals
- O35 - **Dasan M. Thamattoor**, Generation and Trapping of 3-Thiacyclohexyne
- O36 - **Moisés Canle**, In search for truly green photocatalysts
- O37 - **Luis Viegas**, Reactivity of the atmospherically important hydrofluoropolyethers towards OH: a cost-effective implementation of MC-TST

### Supramolecular and Systems Chemistry

#### Session 3c

- IL6 - **Sanzhong Luo**, Stereo-ionic Interaction of Protonated Amines in Asymmetric Catalysis
- O38 - **Ryo Sekiya**, Chemical Functionalization of Nanographene
- O39 - **Florian Auras**, Solvatochromic donor-acceptor covalent organic frameworks
- O40 - **Dirk Kurth**, Metallo-supramolecular polyelectrolytes: From growth kinetics to electrochromic properties
- O41 - **Anna McConnell**, Metal-Organic Cages: Expanding the Toolbox of Stimuli-Responsive Behaviour
- O42 - **Bruno Medronho**, Advances in cellulose dissolution and regeneration: From scattering and rheology to a new NMR approach.

## Thursday

### Physical Foundations of Organic Reactivity

#### Session 1d

- IL8 - **Uta Wille**, Position matters: Amide neighbouring group participation facilitates the rate of phenylalanine oxidation in peptides
- O43 - **Bagrat Shainyan**, Structural, Electronic and Mechanistic Features of Unsaturated Triflamides
- O44 - **Hans-Ullrich Siehl**, The Conundrum of the C<sub>4</sub>H<sub>7</sub><sup>+</sup> Cation Dedicated to George A. Olah
- O45 - **Oliver Maguire**, How to cope with change? The effects of dynamic environments on Out-of-Equilibrium Chemical Reaction Networks
- O46 - **Igor Khmelinskii**, ADH1A - catalysed ATP hydrolysis is coupled to ethanol dehydrogenation by energy transfer

### Reaction mechanisms and Catalysis

#### Session 2d

- IL9 - **María Paz Muñoz**, Precious metal catalysis in Allene chemistry: from divergent systems to heterobimetallic catalysis
- O47- **Satoshi Usui**, In-Cage Reaction of Intermediates Generated in the Photosolvolytic of 3-Substituted-2-benzoyloxy-naphthalene
- O48 - **Luis Frija**, Broad-spectrum Azole-based Molecules: From Strong Ligands in Coordination Chemistry to Organocatalysts
- O49 - **Luis Branco**, Task-Specific Ionic Liquids for CO<sub>2</sub> Capture and Catalytic Conversion in fuels
- O50 - **Bruno S. Souza**, Aminolysis of 1,8-Naphthalic Anhydrides in Aprotic Solvents Involves Two Reaction Paths

### Supramolecular and Systems Chemistry

#### Session 3d

- IL10 - **Adriana Gerola**, Reactive and Selective Supramolecular Artificial Enzymes for Phosphate Transfer Reactions
- O51- **Wataru Setaka**, Thiophenediyl-bridged Macrocages as Crystalline Molecular Dipolar Rotors
- O52 - **Uwe Pischel**, Light-induced Release of Guests from Host-Guest Complexes in Water
- O53 - **Sean Ryan**, Excited Electronic Interactions in Extended Molecular Systems
- O54 - **Carlos Baleizão**, Tuning particle diameter and morphology of hybrid mesoporous silica nanoparticles and application to controlled drug release

Session 3e

IL11- **Shmaryahu Hoz**, A New Reaction Mechanism Diagnostic Tool for the Reaction of SmI<sub>2</sub>

O55 - **Carlos Lima**, Influence of Molecular Symmetry on the Entropy of Pure Phases

O56 - **Ricardo Simões**, Development of novel autoreactive and ecological monocomponent adhesives

O57 - **Manuel Aureliano**, Recent insights into the biological activities of polyoxometalates

O58 - **Francisco José Ostos**, Influence of the surfactant degree of oligomerization on the formation of cyclodextrin:surfactant inclusion complexes