

Wednesday October 12, 2022

CRF-ChemCYS Symposium 2022, 12-14 October

Blankenberge, Belgium

Conference Timetable

Chair

| | | |
|-------|---|-------------------------|
| FM | Functional Materials | Prof. Danny Vanpoucke |
| CB | Chemistry meets Biology | Prof. Ana Cunha |
| CS&M | Chemical Synthesis & Methodologies | Prof. Dirk Vanderzande |
| E&E | Energy & Environment | Prof. Elke Debroye |
| CP&RT | Chemical Processes & Reactor Technologies | Prof. Evelien Baeten |
| R&S | Renewables & Sustainability | Prof. Thomas Heugebaert |

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|-------|----|--|---------------|
| 9:00 | | Registration & Pick-up Room keys | Entrance Hall |
| 10:30 | | Welcome & opening | Auditorium |
| 10:50 | | What is chemistry Europe? Shaun Scally – <i>Wiley</i> | Auditorium |
| 11:05 | P1 | Chemical information: building bridges for chemistry Jonathan Goodman – <i>University of Cambridge</i> | Auditorium |



Wednesday October 12, 2022

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| 11:55 | K1 | Tailored molecular design of organic chromophores – from thermally activated delayed fluorescence to dual-functioning photosensitizers Wouter Maes – <i>UHasselt</i> | Auditorium |
| 12:30 | K2 | Ultrasonic microreactors for chemical manufacturing Simon Kuhn – <i>KU Leuven</i> | Auditorium |
| 13:10 | Lunch & Pick-up Room keys | | Foyer |
| | Auditorium: FM | | Room 2, 3 & 4: CB |
| | | | Room 5: CS&M |
| 14:30 | FM-O1 | Hydrotalcites as effective and selective catalysts for the condensation of small sugars towards the synthesis of polyol-based flame retardants Fatima Rammal <i>KU Leuven</i> | CB-O1 Chemical Evolution Driven by Self-assembly Omer Markovitch <i>University of Groningen</i> |
| | | | CS&M-O1 9-Boratriptycenes: A Lewis Superacids Story Arnaud Osi <i>University of Namur</i> |
| 14:50 | FM-O2 | Phenylpyridine and bipyridine based covalent organic frameworks as metal free photocatalysts for the visible light aerobic oxidation/Povarov cyclization Maarten Debruyne <i>Ghent University</i> | CB-O2 Development of a high-bioanalytical platform for metabolomics Katyeny Manuela da Silva <i>University of Antwerp</i> |
| | | | CS&M-O2 Dearomative Cyclopentannulation of Indoles and Benzofurans Bram Ryckaert <i>Ghent University</i> |

Wednesday October 12, 2022

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| 15:10 | FM- O3 | Synthesis, Characterization and Biological Features of Saponin Based Nanoparticles Cansel Askim Tiryaki <i>Ege University</i> | CB- O3 | Towards the one-pot upgrading of glucose to HMF through hybrid chemo-enzymatic catalysis Marty Kinnaer <i>UC Louvain</i> | CS&M- O3 | 9-phosphatriptycenes as Lewis bases for the frustrated Lewis pair-catalyzed hydrogenation of unactivated olefins: a DFT and experimental study Damien Mahaut <i>University of Namur</i> |
| 15:30 | FM- O4 | Towards stable hybrid perovskites for optoelectronics: designing large organic cations Wouter Van Gompel <i>UHasselt</i> | CB- O4 | Ultralarge Virtual Screening Identifies SARS-CoV-2 Main Protease Inhibitors with Broad-Spectrum Activity against Coronaviruses Andreas Lutgens <i>Uppsala University</i> | CS&M- O4 | Selective imitination of 3-oxo-β-lactams – new route towards 3-amino-β-lactams Sari Deketelaere <i>Ghent University</i> |
| | Room 6: E&E | | Room 13: CP&RT | | Room 14: R&S | |
| 14:30 | E&E- O1 | Industrial decarbonization for the energy transition Talieh Rajabloo <i>UHasselt</i> | CP&RT- O1 | Demystifying the thermodynamics of furfural derivatives aiming at improved separation process design Ilah Joos <i>Ghent University</i> | R&S- O1 | Heat triggered debondable adhesives Tim Maiheu <i>Ghent University</i> |

Wednesday October 12, 2022

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| 14:50 | E&E- O2 | Integrated Direct Air Capture and Electrochemical CO2 Conversion Oriol Gutierrez <i>VITO</i> | CP&RT- O2 | Numerical analysis to reduce axial dispersion with active lateral flow Pierre Gelin <i>Vrije Universiteit Brussel</i> | R&S- O2 | Mechanosynthesis of N-Heterocyclic Carbene Complexes Gianmarco Pisano <i>Ghent University</i> |
| 15:10 | E&E- O3 | Plasma Catalysis for CO2 Hydrogenation: Unlocking New Pathways toward CH3OH Roel Michiels <i>University of Antwerp</i> | CP&RT- O3 | Synthesis of heterogeneous metal oxides catalysts by humid air plasma glidarc: study of the effect of the post-discharge Fanny Hanon <i>UC Louvain</i> | R&S- O3 | Microkinetic analysis of ethylene hydroformylation on a heterogeneous Rh-modified MOF catalyst Sébastien Siradze <i>Ghent University</i> |
| 15:30 | E&E- O4 | Understanding the mechanism of CO2 methanation over MgO-Ni/SiO2 Yufei Xie <i>Ghent University</i> | CP&RT- O4 | Experimental assessment of the ethyl acetate synthesis kinetics by direct addition of ethylene to acetic acid on a silicotungstic acid catalyst Bram Van Wettere <i>Ghent University</i> | R&S- O4 | Lewis acid catalyzed synthesis of methionine hydroxy analogues from tetroses Sergio Calderon-Ardilla <i>KU Leuven</i> |
| 15:50 | Poster Session 1 & Coffe Break | | | | Cafeteria | |
| 17:00 | K3 | Synthetic biology as driving force for biobased production of chemicals using microbial cell factories Eveline Peeters – <i>Vrije Universiteit Brussel</i> | | | Auditorium | |

Wednesday October 12, 2022

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| 17:35 | K4 | Cyclodextrin metal-organic frameworks: from sugars to nanomaterials for biological applications Kristof Van Hecke – <i>Ghent University</i> | Auditorium |
| 18:10 | | Pick-up Room keys | Entrance Hall |
| 19:00 | | Dinner | Restaurant |
| 20:30 | | KaféCV | Cafeteria |

Thursday October 13, 2022

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|-----------|-----------------------|--|---|
| 7:30-9:00 | Breakfast | | Restaurant |
| 9:00 | P2 | Water in coherent light Gerhard Grübel – <i>University of Hamburg</i> | Auditorium |
| 9:50 | K5 | Photo-crosslinkable polymer platform: from bioinks to shape memory polymers Sandra Van Vlierberghe – <i>Ghent University</i> | Auditorium |
| 10:25 | Coffee break | | Foyer |
| 10:55 | K6 | Chemical process development of the Milvexian side chain Ilse Vogels – <i>Janssen Pharmaceutica</i> | Auditorium |
| | Auditorium: FM | | Room 2, 3 & 4: CB |
| 11:30 | FM-O5 | Methacrylate-encapped urethane-based polyesters – influence of backbone and spacer on thermal properties and crosslinking Jasper Delaey <i>Ghent University</i> | CB-O5 Biodegradation of Maleic Anhydride-Grafted Polycaprolactone (PCL-g-MA) with Lipase Kotchaporn Thangunpai <i>University of Tsukuba</i> |
| | | | CS&M-O5 Development of Bulk-Like CdS and CdSe Quantum Dots for Optical Gain Margarita Samoli <i>Ghent University</i> |
| 11:50 | FM-O6 | Crosslinked polyaspartic acid hydrogels as biobased and biodegradable alternative for polyacrylic acid | CB-O6 Reactivity of peroxidases and chlorite dismutases with chlorite and hypochlorite: a spectroscopic |
| | | | CS&M-O6 Design, synthesis and characterisation of novel donor-acceptor combinations affording low voltage losses in |

Thursday October 13, 2022

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| | | <p>Lauren De Grave <i>Ghent University</i></p> | <p>investigation of short-lived intermediates trapped by fast freeze-quenching Ilenia Serra <i>University of Antwerp</i></p> | <p>indoor organic photovoltaics Dries Theunissen <i>UHasselt</i></p> |
| 12:10 | FM-07 | <p>UV -assisted cryogelation of poly(2-oxazoline)s towards supermacroporous hydrogels Tomas Sedlacik <i>Ghent University</i></p> | <p>CB-07 An unbiased approach to exploring biomolecular reactions with hybrid QM/MM Neil McFarlane <i>KU Leuven</i></p> | <p>CS&M-07 Electron microscopic approaches in identifying, understanding & design of catalysts Sreeprasanth Sree Pulinthanathu <i>KU Leuven</i></p> |
| | Room 6: E&E | | Room 13: CP&RT | Room 14: R& |
| 11:30 | E&E-05 | <p>Green Ammonia Synthesis Process with Plasma-driven Nitrogen Oxidation and Catalytic Reduction of Adsorbed NO_x (PNO CRA process) Lander Hollevoet <i>KU Leuven</i></p> | <p>CP&RT-05 Characterization of an acoustic streaming microreactor: uncovering the effect of acoustic streaming on crystallization Cedric Devos <i>KU Leuven</i></p> | <p>R&S-05 Recyclable Polyurethane elastomers via dynamic covalent chemistries Hiba Kassem <i>Ghent University</i></p> |
| 11:50 | E&E-06 | <p>Exploring the reactivity of a Solid Micellar Catalyst (SOMIC) for low-</p> | <p>CP&RT-06 Photometric determination of trace amounts of Al in cc. NaCl solutions used by the</p> | <p>R&S-06 Catalytic pyrolysis of a polyethylene melt with high selectivity to light</p> |

Thursday October 13, 2022

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| | | temperature methanol synthesis Catarina Martins de Brito Mendes <i>Ghent University</i> | | chlor-alkali industry - Coagulation and sedimentation studies Benjamin Csorba <i>Budapest University</i> | | olefins and low coke formation Brent Smeyers <i>KU Leuven</i> |
| 12:10 | E&E-07 | Sustainable Hydrogen from free sunlight and seawater using stabilized plasmonic modified TiO₂ Fons Dingenen <i>University of Antwerp</i> | CP&RT-07 | Characterization of flows in microchannels with scanning 3D μPIV Quentin Galand <i>Vrije Universiteit Brussel</i> | R&S-07 | Sustainable Synthesis of Aromatic Building Blocks via the Upcycling of Polystyrene Based Plastic Waste Yuman Qin <i>University of Antwerp</i> |
| 12:30 | Lunch | | | | Foyer | |
| | Auditorium: FM | | Room 2, 3 & 4: CB | | Room 5: CS&M | |
| 13:50 | FM-08 | Developing design rules for room temperature phosphorescence in solution from purely organic molecules Simon Paredis <i>UHasselt</i> | CB-08 | NMR-based metabolomics reveals a metabolic shift after surgical resection of non-small cell lung cancer Elien Derveaux <i>UHasselt</i> | CS&M-08 | NHC Complexes in Flow (NHC = N-heterocyclic carbene) Andreas Simoens <i>Ghent University</i> |
| 14:10 | FM-09 | Self-assembly behavior of molecules under confinement conditions | CB-09 | Hyphenation of temperature-responsive chromatography and | CS&M-09 | Group IV Metal Oxo Cluster Based Catalysts for |

Thursday October 13, 2022

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| | | | <p>ultrafast chiral chromatography as a generic comprehensive two-dimensional method for the analysis of chiral pharmaceuticals</p> <p>Lihua Yu <i>KU Leuven</i></p> <p>Turaj Rahmani <i>Ghent University</i></p> | <p>the Direct Formation of Amide Bonds</p> <p>Francisco de Azambuja <i>KU Leuven</i></p> |
| 14:30 | FM-O10 | <p>3D printing, where hydrogels and tissue engineering meet</p> <p>Martina Meazzo <i>Ghent University</i></p> | <p>CB-O10</p> <p>Novel Microfluidics Approaches for Selection and Enhancement of Sperm Motility for Improved Fertilization</p> <p>Vyacheslav Misko <i>Vrije Universiteit Brussel</i></p> | <p>CS&M-O10</p> <p>Development of a combined methodology towards mechanistic investigation of rare metal-free, light activated catalysts</p> <p>Andrea Guidetti <i>University of Antwerp</i></p> |
| 14:50 | FM-O11 | <p>Isomeric modulation of thermally activated delayed fluorescence properties in deep-red/near-infrared emitters</p> <p>Sonny Brebels <i>UHasselt</i></p> | <p>CB-O11</p> <p>Development of fluorescent ligands for Voltage-Gated Ion Channels</p> <p>Carlotta Borgarelli <i>KU Leuven</i></p> | <p>CS&M-O11</p> <p>Synthesis of bridged bicyclic nitrogen scaffolds via orthogonal tandem catalysis</p> <p>Marjo Waeterschoot <i>University of Antwerp</i></p> |
| | Room 6: E&E | | Room 13: CP&RT | Room 14: R&S |

Thursday October 13, 2022

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| 13:50 | E&E-08 | Techno-economic model for the application potential of hydrogen storage technologies Lucas Hanssens <i>KU Leuven</i> | CP&RT-08 | Exploration of Catalytic Pyrolysis with Active Learning Yannick Ureel <i>Ghent University</i> | R&S-08 | A green analytical method to characterize unsaturated hydrocarbons in waste polyolefin pyrolysis oil using FT-IR Trang Thi Bui <i>University of Antwerp</i> |
| 14:10 | E&E-09 | Catch the Heat! Ionut Tranca <i>Vrije Universiteit Brussel</i> | CP&RT-09 | Electrochemical conversion of CO₂ to formic acid at elevated temperatures Alana Rossen <i>University of Antwerp</i> | R&S-09 | Use of FTIR microspectroscopy to assess the extraction viability of food waste Paula Varas Perez <i>UHasselt</i> |
| 14:30 | E&E-010 | Innovative battery materials: it's all about chemistry! Dries De Sloovere <i>UHasselt</i> | CP&RT-010 | Enabling Flow synthesis of zeolites Dries Vandenamee <i>KU Leuven</i> | R&S-010 | 3D Investigation of Nanoparticle Assemblies by Electron Tomography Safiyye Kavak <i>University of Antwerp</i> |
| 14:50 | E&E-011 | Technical and Economical Aspects of Advanced Biofuel Production and Separation Keikhosro Karimi <i>Vrije Universiteit Brussel</i> | CP&RT-011 | Microfluidic magnetic platform for repetitive coating of particles Amaury de Hemptinne <i>Vrije universiteit Brussel</i> | R&S-011 | Fresh water production from atmospheric air: Technology and innovation outlook Robin Peeters <i>KU Leuven</i> |
| 15:10 | Poster session 2 & Coffee break | | | | Cafeteria | |

Thursday October 13, 2022

| | Auditorium: FM | Room 2, 3 & 4: CB | Room 5: CS&M |
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| 16:20 | FM-O12 Turning 3D-COFs into luminescent ratiometric thermometers Laurens Bourda <i>Ghent University</i> | CB-O12 Immobilizing neuroglobin in mesoporous materials – monitoring protein structure and dynamics with spin-label electron paramagnetic resonance Lore Van Den Bergh <i>University of Antwerp</i> | CS&M-O12 Synthesis and structural characterization of phosphate-based geopolymers Marko Rukavina <i>University of zagreb</i> |
| 16:40 | FM-O13 Controlled self-assembly of molecular motors and switches at the solution/solid interface: Towards light induced coherent rotary motion Robby Reynaerts <i>KU Leuven</i> | CB-O13 Effect of membrane curvature and lipid composition on membrane permeability in liposomal drug delivery Samaneh Davoudi <i>Ghent University</i> | CS&M-O13 Construction of M-C and M-N bonds: "Golden" synthons, materials, pre-catalysts and mechanistic probes Nikolaos Tzouras <i>Ghent University</i> |
| | Room 6: E&E | Room 13: CP&RT | Room 14: R&S |
| 16:20 | E&E-O12 Characterization of degradation products from Advanced Oxidation Processes using Temperature Responsive Comprehensive LCxLC-HRMS | CP&RT-O12 On the Relevance of Molecular Machine Learning in Industrial Chemistry | R&S-O12 An experimental study on the optimization of process parameters for super-dry reforming of methane |

Thursday October 13, 2022

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| | Elena Bandini <i>Ghent University</i> | Maarten Dobbelaere <i>Ghent University</i> | Michiel Van Cauwelaert <i>Ghent University</i> |
| 16:40 | E&E- O13 Identification of synthetic antioxidants in consumer products through LC-QTOF-MS Maarten Roggeman <i>University of Antwerp</i> | CP&RT- O13 CFD – Study for Enhanced Degassing of a Dehydrogenation Reactor for Liquid Organic Hydrogen Carriers Laurens Van Hoecke <i>University of Antwerp</i> | R&S- O13 Acidity and metal ratio effects on the low temperature hydrodeoxygenation of anisole over NiCu on SiO₂ and γ-Al₂O₃ Tom Vandevyvere <i>Ghent University</i> |
| 17:00 | K7 How can techno-economic and techno-sustainability assessment contribute to chemical research? Steven Van Passel – <i>University of Antwerp</i> | | Auditorium |
| 17:35 | K8 Impact chemicals strategy for sustainability on chemical research and development Kristel Bernaerts – <i>KU Leuven</i> & Tine Cattoor – <i>Essencia</i> | | Auditorium |
| 18:10 | Group picture | | In front of venue |
| 19:30 | Aperitif | | Cafeteria |
| 20:00 | Dinner | | Restaurant |
| 22:00- 3:00 | Live performance by Totally Soul | | Cafeteria |

Friday October 14, 2022

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| 8:00-9:30 | Breakfast | | Restaurant | |
| 9:30 | K9 | Towards a climate neutral chemical industry in Europe: governance & policy <i>Sebastian Oberthur – Vrije Universiteit Brussel</i> | Auditorium | |
| | Auditorium: FM | Room 2, 3 & 4: CB | Room 5: CS&M | |
| 10:05 | FM-O14 | Light-Stabilized Dynamic Materials: Tuning the Dynamic Character <i>Alyssa Ghielmetti Ghent University</i> | CB-O14 The Notorious Z.B.G.: Synthesis and Biological Evaluation of Potent HDAC6 Selective Inhibitors with a Non-Hydroxamic Acid Zinc Binding Group to Overcome Therapeutic Limitations <i>Silke Geurs Ghent University</i> | CS&M-O14 Selective Nickel-Catalyzed Hydrodeacetoxylation of Aryl Acetates <i>Gilles De Smet University of Antwerp</i> |
| 10:25 | FM-O15 | Bio-inspired mineralization of CO₂ to functional CaCO₃: effect of different CO₂ absorption promotor and crystal growth modifier <i>Dharmjeet Madhav</i> | CB-O15 Solid-phase peptide synthesis, folding and biological characterization of carboxyterminally truncated human CXC chemokine ligand 10 CXCL10(1-73) <i>Luna Dillemans</i> | CS&M-O15 Transformations of phosphonochloridates to phosphonates and phosphonamidates under mild coupling conditions <i>Simon Backx</i> |

Friday October 14, 2022

| | <i>KU Leuven</i> | | <i>KU Leuven</i> | | <i>Ghent University</i> | |
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| | Room 6: E&E | | Room 13: CP&RT | | Room 14: R&S | |
| 10:05 | E&E-O14 | Lignin-Supported Heterogeneous Photocatalyst for the Direct Generation of H₂O₂ from Seawater Peng Ren <i>University of Antwerp</i> | CP&RT-O14 | Enhancing CO₂ conversion by plasma reactor in series Rani Vertongen <i>University of Antwerp</i> | R&S-O14 | Let the sun do your chores! Hannelore Peeters <i>University of Antwerp</i> |
| 10:25 | E&E-O15 | Template synthesis of fibrous catalysts for environmental application Maximiliano Rodriguez <i>UC Louvain</i> | CP&RT-O15 | Ray tracing-assisted optimization of light absorption in gas-liquid flow photosensitized oxidations Anca Roibu <i>KU Leuven</i> | R&S-O15 | Improved induction adsorptive CO₂ capture process Mohsen Gholami <i>Vrije Universiteit Brussel</i> |
| 10:45 | Coffee Break | | | | Foyer | |
| | Auditorium: FM | | Room 2, 3 & 4: CB | | Room 5: CS&M | |
| 11:15 | FM-O16 | Fine-tuning the endcap chemistry of acrylated poly(ethylene glycol)-based hydrogels for the treatment of burn wounds | CB-O16 | Photo-alkylation of DNA secondary structures, exploiting photosensitizer and ligand co-localization: from structure-selectivity towards sequence-specificity | CS&M-O16 | Defective UiO-66 metal-organic frameworks as aldol reaction catalysts: Impact of surface defects on activity and selectivity |

Friday October 14, 2022

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| | | Manon Minsart <i>Ghent University</i> | | Enrico Cadoni <i>Ghent University</i> | | Noor Aljammal <i>Ghent University</i> |
| 11:35 | FM-O17 | Rhodium anchored onto a covalent triazine framework as heterogeneous catalyst for transfer hydrogenation of N-heterocycles in water Jonas Everaert <i>Ghent University</i> | CB-O17 | Chromium Toxicity: The role of Analytical Chemistry in Exposure to Chromium Jelle Verdonck <i>KU Leuven</i> | CS&M-O17 | Aluminium and Acid Site Diversity during Zeolite Crystallization and Thermal Activation Julien Devos <i>KU Leuven</i> |
| 11:55 | FM-O18 | Unravelling the performance of Pt-Ni ORR electrocatalysts by combining electrochemical with advanced TEM studies Sven Arnouts <i>University of Antwerp</i> | CB-O18 | A simple model for the Pauli Repulsion with utility in QM, MM and Chemical Education Jordy Peeters <i>Vrije Universiteit Brussel</i> | CS&M-O18 | Catalyst-free solution polymerization of poly(alkylene terephthalate)s: towards high molar masses and molar mass control Lenny Van Daele <i>Ghent University</i> |
| | Room 6: E&E | | Room 13: CP&RT | | Room 14: R&S | |
| 11:15 | E&E-O16 | Modeling Realistic Catalyst Nanoparticles for Fischer-Tropsch Synthesis using Machine Learning Potentials | CP&RT-O16 | Innovative Au-Sn-SiO₂ bifunctional material for the upgrading of glycerol to methyl lactate | R&S-O16 | Screening of biomass residue streams for their applicability as feedstocks for activated carbon production and their compliance as electrode material |

Friday October 14, 2022

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| | Konstantijn Rommens <i>Ghent University</i> | Margot Van der Verren <i>UC Louvain</i> | Willem Vercruyssen <i>UHasselt</i> |
| 11:35 | E&E-017 Effect of pH cycling and background ions on the formation of stable magnesium carbonate at low temperature Veerle Vandeginste <i>KU Leuven</i> | CP&RT-017 Catalytic dehydration of 1,3-Butanediol into 1,3-Butadiene Ghinwa Fayad <i>KU Leuven</i> | R&S-017 Sodium aluminate-based materials as promising catalysts for biodiesel production Giovanni Pampararo <i>UC Louvain</i> |
| 11:55 | E&E-018 Unravelling the mysteries of arsenic in the Zenne River (Belgium): sources, distribution, geochemistry, and bioavailability Vendula Smolikova <i>Vrije Universiteit Brussel</i> | CP&RT-018 Perspectives of continuous heterogeneously catalyzed hydroformylation of large olefins Maria Manzano Herrero <i>Ghent University</i> | R&S-018 NMRCoRe@CMWS as a node of convergence in molecular water science in Flanders Eric Breynaert <i>KU Leuven</i> |
| 12:15-13:30 | Lunch | | Restaurant |
| 13:30 | P3 The new chemist Javier Garcia Martinez – <i>IUPAC President</i> | | Auditorium |
| 14:30 | The Human Link Stress-less(s): coping with stress in an academic environment <i>ROOM 5</i> | Scimingo Time to reach out! A crash course on scientific communication <i>ROOM 2, 3 & 4</i> | |

Friday October 14, 2022

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| 15:40 | Start Closing Ceremony | Auditorium |
| 15:50 | Chemistry Europe Fellows Award Tatjana Parac-Vogt <i>KU Leuven</i> | Auditorium |
| 15:55 | Incentive Awards C.G.B.-C.B.B. Roy Lavendomme – <i>Ghent University &</i> Ruben Van Lommel – <i>KU Leuven/ Vrije Universiteit Brussel</i> | Auditorium |
| 16:10 | Poster and Oral Contribution Awards | Auditorium |
| 16:45 | Final Word | Auditorium |
| 16:50 | End of CRF-ChemCYS symposium 2022 | Auditorium |