Programme NCCC 2025

Requested: 2025-03-26 10:03

	Monday: March 10th			
10:45 - 11:00	Opening NCCCXXVI by Atsushi Urakawa and Caroline Paul (Rotonde)			
11:00 - 11:50	**PL1** *T. Laino – IBM Research Europe* Fueling the Digital Chemistry Revolution with Language and Multimodal Foundation Models chaired by A. Urakawa (TUD)			
11:50 - 13:00	Lunch Break			
	Rotonde	**Sorbonne**	**Boston 17-19**	**Cambridge 30**
	Electrocatalysis chaired by R. Kortlever (TUD)	Heterogeneous catalysis - CO2 hydrogenation chaired by J. Xie (RUG)	Organic chemistry and organo/biocatalysis chaired by J. Reek (UvA)	Characterisation and operando studies chaired by N. Kosinov (TU/e)
13:00 - 13:20	**O1** Membraneless Electrolyzers: A Viability Study from Cell to Stack in Comparison with Commercial Systems *Dr. Borah – University of Antwerp*	**O2** Constructing inverse CeOx/Co catalysts for enhanced low-temperature CO2 hydrogenation *Y.G Gao – Eindhoven University of Technology*	**O3** Identifying peptide catalysts for Pictet-Spengler reactions via phage display *I.D. Jansen – University of Groningen*	**O4** Spatiotemporal X-Ray Absorption Spectroscopy of Ni-Mg-Al Mixed Oxide Catalysts During Dry Methane Reforming *S Ferwerda – Utrecht University*
13:20 - 13:40	**O5** Toluene hydrogenation using zero-gap PEM electrolyzer: Strategies to achieve high conversions *E. Demiröz – Delft University of Technology*	**O6** CO2 conversion over a Ru-based dual functional material for CO2 capture and conversion and its dependence on Ru-alkali metal interactions *F. Karaçoban – Wageningen University and Research Centre*	**O7** Asymmetric Enantio-Complementary Synthesis of Thioethers via Ene-Reductase Catalysed C-C bond formation *C. Heckmann – Delft University of Technology*	**O8** In Situ EC-STM Study of a Roughening Gold Single-Crystal Electrode Surface by Oxidation-Reduction Cycles in Different Electrolytes *S. Behjati – Leiden University*
13:40 - 14:00	**O9** Manufacturing multiscale porous electrodes with non-solvent induced phase separation for high performance redox flow battery electrodes *B. Liu – Eindhoven University of Technology*	**O10** Spark ablation: a dry, physical, and continuous method to prepare powdery heterogeneous catalysts for CO2 methanation *P. Hongmanorom – UCLouvain*	**O11** Nature-Inspired Rhythmic Processes: A Novel Route Towards Materials *S.A. Runikhina – University of Groningen*	**O12** The Electro-Oxidation of β-O-4 Model Compounds monitored in a Chamber-Separated Cell using In Situ ATR-IR Spectroscopy *S.M.K. Schwartmann – Utrecht University*
14:00 - 14:20	**O13** Cation effects on caffeinated-Pt single crystal surfaces in alkaline HER	**O14** Influence of Hydrophobic and Hydrophilic Carbon Supports on Iron-based Catalysts for High-Pressure Low-Temperature Reverse Water Gas Shift *W.M. Meng – University of Groningen*	**O15** Integrated Strategy for Mild Catalytic Lignin Valorization: Selective Production of Aromatic Benzoquinones from Lignocellulosic Biomass *G. Guo – University of Groningen*	**O16** Advanced Sample Preparation for Total Reflection X-ray Fluorescence Spectroscopy for a Correlative Micro-spectroscopic Approach *K.B. Siebers – Utrecht University*
14:20 - 14:40	Coffee break			

	Rotonde	Sorbonne	Boston 17-19	Cambridge 30
	Materials chemistry chaired by A. Bansode (TUD)	Electrocatalysis - fine chemicals chaired by A. Garcia (UvA)	Biocatalysis chaired by I. Drienovska (VU)	Photocatalysis chaired by K. Wenderich (UT)
14:40 - 15:00	**KN1** Diffusion in nanoporous materials: The need for speed in measurements and applications *R. Ameloot – Katholieke Universiteit Leuven*	**O17** Sustainable electrocatalytic reductive animation of levulinic acid *M. Grundmann – RWTH Aachen University*	**O18** Metal dependent activity of cupin enzymes *H. Brasselet – Delft University of Technology*	**O19** On the Effect of Light on the CO Intermediate during CO2 Hydrogenation over a Co/TiO2 Catalyst *D.N. Maaskant – Utrecht University*
15:00 - 15:20		**O20** Electrocatalytic C-H Amination from Primary Amines *D.D. Snabilié – University of Amsterdam*	**O21** Asymmetric Au(I)-Enzymatic Catalysis *F. Della-Felice – University of Groningen*	**O22** In-situ X-ray absorption spectroscopy study of the deactivation mechanism of a Ni-SrTiO3 photocatalyst slurry active in water splitting *M.T. Abudukade – University of Twente*
	Rotonde	**Sorbonne**	**Boston 17-19**	**Cambridge 30**
	Safety in chemical catalysis chaired by A. Bonsode (TUD)	Electrocatalysis chaired by A. Garcia (UvA)	Bruker workshops	VIRAN-NIOK session (for the members of VIRAN & NIOK)
15:20 - 15:40	**O23** Learnings from a reactor explosion: Towards safer start-ups of catalysts systems by Willem Groendijk - Shell	**O24** Titanium Carbide Hollow Fiber Electrodes: A Feasible Alternative for Platinized Titanium Hollow Fibers? *T. de Koning Gans – University of Twente*	Breaking New Ground in Catalysis and Spectroelectrochemistry: the new Vertex NEO-R FT-IR spectrometer by M. Kessler	A new national catalysis roadmap – status and way forward
15:40	Learnings from a reactor explosion: Towards safer start-ups of catalysts systems by Willem Groendijk - Shell	**O25** Electric double layer at stepped Pt/water interface: insights from AIMD and continuum modeling *J Liu – Leiden University*	Raman microscopy for the spatial characterization of catalysts and catalytic reactions by F. Knechtel	A new national catalysis roadmap – status and way forward
16:10 - 18:10	Poster session A (Erasmus)			
18:10 - 20:15	Dinner, with presentation of Dutch Catalysis Roadmap (CoI - VIRAN+NIOK) (Atrium)			
20:15	CDO Session (Rotonde) and KNCV career coaching (Room B9)			
	Tuesday: March 11th			
09:00 - 09:50	**PL2** N3C Award lecture chaired by C. Paul (TUD)			
	Rotonde	**Sorbonne**	**Boston 17-19**	**Cambridge 30**
	Materials chemisty chaired by M.F.N d'Angelo (TU/e)	Heterogeneous catalysis - mechanism and kinetics chaired by M. Monai (UU)	Electrocatalysis chaired by P. Ngene (UU)	Characterisation and operando studies chaired by A. van Blaaderen (UU)

09:50 - 10:10	**O26** 3D Morphology Evolution of γ-Al2O3 Pores during Catalyst Preparation *J.M.J.J. Heinrichs – Eindhoven University of Technology*	**O27** Unravelling the role of lattice strain on the prototypical hydrogen-deuterium exchange reaction *J.P. Jonasse – Utrecht University*	**O28** Electrocatalytic CO(2) reduction to Methanol on Pt(111) modified with a Pd Monolayer *A. Wawrzyniak – Leiden University*	**O29** Mechanistic insights into Direct Air Capture with carbon supported K2CO3 sorbents using In Situ XRD *T.G. de Groot – Wageningen University and Research Centre*
10:10 - 10:30	**O30** Airborne preparation of Cu based heterogeneous catalysts: Structural features and catalytic competitiveness *G. Pampararo – Katholieke Universiteit Leuven*	**O31** Lignin depolymerization kinetics simulations through continuous lumping: mechanistic features in relation to β-O-4 bond cleavage *L.G. Garbarino – Ghent University*	**O32** Demonstration of confinement and voltage homogeneity for stable CO2 electrolysis on copper electrodes *J. Kok – Delft University of Technology*	**O33** Establishing Sample Preparation Protocols to Facilitate Accurate Nanoplastic Characterization *L.M. Zoutendijk – Utrecht University*
10:30 - 10:50	Coffee break			
	Rotonde	**Sorbonne**	**Boston 17-19**	**Cambridge 30**
	Biocatalysis chaired by C. Mayer (RUG)	Heterogeneous catalysis - CO2 conversion chaired by P.P. Pescarmona (RUG)	Electrocatalysis chaired by M. Koper (U. Leiden)	Computational chemistry and data science chaired by E.A. Pidko (TUD)
10:50 - 11:10	**KN2** Harnessing the catalytic power of nitrogen-nitrogen bond forming enzymes for sustainable chemical synthesis *S. Schmidt – University of Groningen*	**O34** Sustainable catalytic synthesis of fully renewable cyclic carbonates *G. Berluti – University of Groningen*	**O35** Modular Design of Cu-S Planar Building Units in a Metal-Organic Framework for Enhanced Selectivity in Electrochemical CO2-to-Formate Conversion *K. Roohi – Delft University of Technology*	**O36** From Catalyst Design to Reaction Testing in CO_2 Valorization: Harnessing Big Data for Structure-Activity Correlation *J.A. Mendoza Mesa – Katholieke Universiteit Leuven*
11:10 - 11:30		**O37** Role of Zn in enhancing CO2 hydrogenation to methanol over ZnxZrOy catalysts *Z. Zanganeh – Ghent University*	**O38** Unveiling Dual Roles of Organic Cations in Alkaline Hydrogen Evolution Reaction: From Promotion to Suppression *J. Fernández-Vidal – Leiden University*	**O39** Homogeneous Catalyst Design in the Digital Age: Insights from Machine Learning and Data Representation *A.V. Kalikadien – Delft University of Technology*
11:30 - 11:50	**O40** Biocatalytic Cascades: From geraniol to enantiopure (R)-citronellal *C. Ferrer Carbonell – Delft University of Technology*	**O41** Elucidating the Factors that Determine the Activity and Stability of In2O3-based Catalysts in CO2 Hydrogenation *M. Becker – ETH Zürich*	**O42** Role of pH in the electrochemical reduction of aldehydes and formose-like reactions *A. Raman – University of Twente*	**O43** A DFT Study of the promotion of Pd/CeO2 for CO oxidation by Surface Lattice Doping *M. Li – Eindhoven University of Technology*
11:50	Lunch break			
13:00 - 13:50	**PL3** *P. Melchiorre – University of Bologna* Photochemistry, Organocatalysis & Enzymes: New Radical Opportunities chaired by B. de Bruin (UvA)			
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	Heterogeneous	Electrocatalysis chaired	Photocatalysis and organic	Heterogeneous

	catalysis - methane activation chaired by E.T.C. Vogt (UU)	by M.C. Figueiredo (TU/e)	chemistry chaired by D. Hetterscheid (U Leiden)	catalysis - Reaction mechanism chaired by I. Vollmer (UU)
13:50 - 14:10	**KN3** Demonstration and scale-up of autothermal oxidative coupling of methane to produce olefins by Pankaj Gautam (SABIC)	**O44** Salt Formation and Flooding in MEA Cells for CO2 Electrolysis under Industry-Relevant Temperatures *H.M. Pelzer – Delft University of Technology*	**O45** Preorganization within Photoactive Pt12L24 Nanospheres for Accelerated Decarboxylation Catalysis at Low Concentrations *R. Ham – University of Amsterdam*	**O46** The Role of Water in Copper Zeolite Methane Oxidation *M.L. Bols – Ghent University*
14:10 - 14:30		**O47** Kinetic Analysis of the Oxygen Reduction Reaction Electrocatalysis Using Advanced Transient Voltammetry *R.Z. Sol – Leiden University*	**O48** Photoenzymatic biaryl formation by dual Ni/aryl ketone cross coupling *T.C. Böllersen – University of Groningen*	**O49** Detection of Hydroxylamine Intermediate Opens a New Perspective on Ammonia Selectivity in Metal-Catalyzed Nitrate Reduction *J. Betting – University of Twente*
14:30 - 14:50	**O50** Developing a Two-Stage Thermocatalytic Process to Convert CO2 into Aromatics *J.J.G. Kromwijk – Utrecht University*	**O51** On the effect of support polarity in carbon-supported nickel nanoparticles for electrocatalytic hydrogen peroxide production *I.J. van Luijk – Wageningen University and Research Centre*	**O52** Enantioselective intramolecular cyclization of 2,3-dihydrobenzofurans using strong photoreductants *C.J. Nielsen – University of Amsterdam*	**O53** Tracking Iron Dynamics in NH3-SCR Catalysis: Mechanistic Insights gained by Quasi In-Situ Mössbauer Spectroscopy *D.G.J. Broens – Eindhoven University of Technology*
14:50	Coffee break			
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	Coordination chemistry chaired by J.C. Slootweg (UvA)	Heterogeneous catalysis - depolymerisation chaired by F.J. de Zwart (ETHZ)	Electrocatalysis - in situ/operando study chaired by W. van der Stam (UU)	Homogeneous catalysis chaired by M.E. Moret (UU)
15:10 - 15:30	**O54** Metal-Ligand Proton Tautomerism: The Hidden Role of Tunneling *S. Melnikov – Utrecht University*	**O55** Mechano-Catalytic Depolymerization of Polypropylene by Fracture of Covalent Materials *A. Hergesell – Utrecht University*	**O56** Protochips electrocatalysis at realistic temperatures using liquid phase electron microscopy - N.A. Krans – Protochips	**O57** Controlled homogeneous monohydrogenation of muconic acid and muconates via Ru catalyzed transfer hydrogenation *L. De Vriendt – Katholieke Universiteit Leuven*
15:30 - 15:50	**O58** Cavity-Directed Synthesis of Labile Polyoxometalates for Catalysis in Confined Spaces *C. Liu – Katholieke Universiteit Leuven*	**O59** Catalytic pyrolysis: paving the way for circular polyurethane *T.G.W. Engels – University of Groningen*	**O60** Tracking the surface structure and the influence of cations and anions on the double-layer region of a Au(111) electrode *A. Adnan – Leiden University*	**O61** Homogenously catalyzed additive-free formic acid dehydrogenation assisted by “Hidden” metal-ligand cooperation *S. Shi – University of Amsterdam*
15:50 - 16:10	**KN4** Redox-active formazanate ligands in coordination chemistry and applications *E. Otten – University of Groningen*	**O62** Investigating influence of Ni particle size on hydrogenolysis of PE *V. Drozhzhin – Eindhoven University of Technology*	**O63** Quasi simultaneous X-ray absorption and diffraction to study activation and regeneration of an indium-bismuth catalyst for CO2 electroreduction at high current density *M. Biggiero – Utrecht*	**O64** Manganese(I)-Catalyzed Enantioselective alkylation to access P-stereogenic phosphines *B. Wan – University of Groningen*

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16:10 - 16:30		**O65** Chemical Recycling of HDPE and LDPE from Municipal Waste Stream Using Hydrothermal Liquefaction Process *S. Chien – University of Amsterdam*	**O66** Surface Restructuring of Copper Electrode during CO2 Electro-reduction Revealed by In Situ Electrochemical Atomic Force Microscopy *H. Wang – Utrecht University*	**O67** Highly Strained Tricyclic Oxanorbornenes with Uncommon Reactivity Enable Rapid ROMP for High-Performance Polyenes *B.O. Grabbet – Utrecht University*
16:30	Poster session B (Erasmus)			
18:30	Dinner (Atrium)			
20:00	Bowling tournament			
	Wednesday: March 12th			
09:00	**PL4** *SB Bals – University of Antwerp* Transmission electron microscopy to understand the behavior of nanomaterials during catalysis chaired by P.E. de Jongh (UU)			
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	Electrocatalysis chaired by D.M. Morales (RUG)	Heterogeneous catalysis - ammonia chaired by J.A. Faria (UT)	Electrocatalysis - mechanism chaired by R.V. Mom (U Leiden)	Sustainability and Photochemistry chaired by T. Bouwens (TUD)
09:50 - 10:10	**KN5** Electrocatalytic synthesis of fertilizers *M. Costa Figueiredo – Eindhoven University of Technology*	**O68** Metal Hydride Nanocomposite Materials as TM-free Catalysts for Ammonia Synthesis *J.C. Verschoor – Utrecht University*	**O69** Operando Spectroelectrochemistry Elucidates the Mechanism of Molecular Electrocatalytic CO2 Reduction Catalyzed by an Iron Porphyrin *A. Salamé – Leiden University*	**O70** High-Tech Innovations for Low-Tech Solutions: Implementing Golden Hydrogen for Off-Grid Clean Cooking and Cooling *M Michiels – Katholieke Universiteit Leuven*
10:10 - 10:30		**O71** A Century of Data: Thermodynamics and Kinetics for Ammonia Synthesis on Various Commercial Iron-based Catalysts *H Keestra – University of Twente*	**O72** Cation-mediated pseudocapacitance dominates the interfacial charging of α-Fe2O3(0001) in alkaline electrolyte *J.J.J. Eggebeen – Leiden University*	**O73** Reversible metal-binding with the flick of a light switch *L. Stringer – Utrecht University*
10:30	Coffee break			
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	Computational chemisry in catalysis chaired by G. Li (WUR)	Electrocatalysis chaired by M. Altomare (UT)	Heterogeneous catalysis - bio-based materials conversion chaired by J.H. Bitter (WUR)	Photocatalysis chaired by G. Mul (UT)
10:50 - 11:10	**KN6** Theory-Driven Innovation in Single Atom Alloy Catalysis: from Data and Models to Understanding and Design *M. Stamatakis – University of Oxford*	**O74** Direct growth of nickel borides on Ni foam for enhanced electrocatalytic performance in the oxidation of 5-hydroxymethylfurfural *J. Hong – University of Groningen*	**O75** Maximising cyclopentanone yields from furfural hydrogenation via catalytic and reactor synergy *A.S. Patil – Eindhoven University of Technology*	**O76** Thermal-photocatalytic coupled regeneration of activated carbon filters for indoor air VOC abatement. *K.S Schoofs – University of Antwerp*
11:10 -		**O77** Hybrid Electrolyzer Configuration for	**O78** Selective production of biobased primary amines by	**O79** New Mechanochemical

11:30		Efficient CO2 Electrolysis *A.M. Ismail – Delft University of Technology*	reductive amination over atomically dispersed Pt1/S-C *Y. Ding – Wageningen University and Research Centre*	Synthesis of Covalent Triazine-based Frameworks for the Photocatalytic Production of H2O2 *L.S. Häser – RWTH Aachen University*
11:30 - 11:50	**O80** First-Principles Insights into the Catalytic Activity of Pd and Pt Across Size Scales with the Promoting Effect of Ceria Support *S.W. Bernart – Eindhoven University of Technology*	**O81** The potential-dependent structure of Pt3Ni alloy electrocatalysts and its effect on electrocatalytic activity *H.J. Nagra – Leiden University*	**O82** The effect of Ag addition to Au catalysts for the oxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic acid *H.L. Nolten – Utrecht University*	**O83** Defect-Engineered Core-Shell Au@TiO_2 Photocatalysts for Enhanced Visible-Light CO_2 Conversion *A. Raes – University of Antwerp*
11:50 - 12:10	**O84** General Trends in the Composition-Activity Relations in High-Entropy Alloys *V.A. Mints – Imperial College*	**O85** Ultrathin Overlayers for Anode Protection in Offshore Green Hydrogen Production via Saline Water Electrolysis *K.S. Encalada Flores – Delft University of Technology*	**O86** Effect of Support Acidity for Acrolein Synthesis by Glycerol Dehydration over WO3/TiO2: N, S and P Doping *M. Battisti – RWTH Aachen University*	**O87** Evaluation of TiO2 photocatalytic coating on metallic substrates: influence of substrate type, coating layers, and operational conditions *D.B. Baetens – University of Antwerp*
12:10 - 13:10	Lunch break			
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	Computational chemistry chaired by N. Artrith (UU)	Atomically-defined solid catalysts chaired by M. Saeys (Ghent U)	Electrocatalysis chaired by K. Wenderich (UT)	Homogeneous catalysis chaired by E. Otten (RUG)
13:10 - 13:30	**O88** Using DFT-based Molecular Dynamics to Understand the Mechanism of COx-to-Methonal in Cobalt Complex Electrocatalysis *L.Z. Zhuo – University of Amsterdam*	**O89** Design of phosphine based solid molecular catalysts for the telomerization of isoprene with various nucleophiles *J. Nikodemus – RWTH Aachen University*	**O90** Modifying a carbon-based gas diffusion layer for electrochemical CO2 reduction to multi-carbon products in acidic electrolyte *K.M.R. Lawrence – Delft University of Technology*	**O91** Oxidative conversion of cellulose-derived furanic compounds to furan-2,5-dicarboxylic acid *A.R.H. Kenbeek – University of Amsterdam*
13:30 - 13:50	**O92** Sulfur-centered Lewis superacid on sulfated zirconium oxide enables the degradation of the polyolefins *A.A. Kolganov – Delft University of Technology*	**O93** Exploring the stability of Ru(III) single-sites in amorphous silica: a selective catalyst for CO2 hydrogenation to formate *S. Santos – Ghent University*	**O94** On the Relevance of Surface Hydroxyl Groups in Carbon Catalysts for the Electrocatalytic Production of H_2O_2 *P. Mazaira Couce – Wageningen University and Research Centre*	**O95** Schrock type Metathesis Catalysts: When a Nobel Prize Award Becomes an Industrial Reality *E. Robe – XiMo Hungary*
13:50 - 14:40	**PL5** Scale-down studies for biocatalysis by John Woodley (DTU) chaired by R. Leveson-Gower (TUD)			
14:40 - 15:00	Prizes & Closure (Rotonde)			
15:00	Buses to Leiden Central Station			