

| Monday March 2 |  |  |  |  |
|----------------|--|--|--|--|
| 10.45          | Opening NCCC X (Rotonde)   |  |  |  |
| 11.00          | <b>P1</b> Molecular Foundations of Heterogeneous Metal Catalysis Prof. dr. Gabor A. Somorjai - University of California, Berkeley, USA   |  |  |  |
| 11.45          | <b>P2</b> Metal-Ligand Cooperation in Bond Activation and New Catalysis Prof. Dr. David Milstein - Weizman Institute of Science, Revohot, Israel   |  |  |  |
| 12.30          | Lunch (12.30-13.45)<br>Poster session I: Posters with even serial numbers (Asamblea, Alegria and Oxford 18)  |  |  |  |
|                | Rotonde  | Sorbonne 2   | Cambridge 32   | Cambridge 30   |
|                | <b>Homogeneous Catalysis</b>   | <b>Heterogeneous Catalysis</b>   | <b>Tools: Theory, Spectroscopy and Model Catalysts</b>   | <b>Sustainable Chemistry, Energy &amp; Devices</b>   |
| 13.45          | 1 Ruthenium-diphosphine Cp complexes as catalysts for the allylation of phenols with allyl alcohol; relation between structure and selectivity<br><i>J. A. van Rijn Leiden University</i>              | 5 On the role of CO <sub>2</sub> in the total oxidation of propane over a CuO-CeO <sub>2</sub> /Al <sub>2</sub> O <sub>3</sub> catalyst<br><i>V. Balcaen Gent University</i> | K1<br><br>Frontiers in multi-scale catalysis modeling<br><br>Dr. Karsten Reuter - Fritz-Haber-Institut Berlin, Germany   | 13 Experimental and modeling analysis of catalytic reforming of methane to hydrogen in an adsorption enhanced fixed bed reactor<br><i>M.H. Halabi TU/e</i> |
| 14.10          | 2 Lewis Acid-Controlled Regioselectivity in Styrene Hydrocyanation<br><br><i>Bini, L. B., TU/e</i>   | 6 The direct production of methanol over Cu-ZSM-5 zeolites: A quantitative structure-performance relationship<br><br><i>N.V. Beznis University of Utrecht</i>                |  | 14 Application of Salts as Catalysts for the Conversion of Glucose to HMF and Levulinic Acid<br><br><i>C.B. Rasrendra Rijksuniversiteit Groningen</i>      |
| 14.35          | 3 Single hydrogen bonds to form Supramolecular heterobidentate ligands and for substrate orientation: application in asymmetric hydrogenation<br><br><i>Breuil, PAR, University of Amsterdam, HIMS</i> | K2<br><br>From fundamental insights towards practical catalysts - nanostructured carbons in catalysis<br><br>Dr. Harry Bitter - University of Utrecht                        | 9 Symmetric transition state analysis in computational catalysis<br><br><i>Bouke Bunnik TU/e</i>   | 15 Catalytic Glycerol Conversion into 1,2-Propanediol in Absence of Added Hydrogen<br><br><i>Sels B. F. Catholic University of Leuven</i>                  |
| 15.00          | 4 Homogeneous hydrogenation of Olefins and Alkynes Using Iron Nanoparticles as Catalyst<br><br><i>Pim Huat Phua DSM</i>  |  | 10 Haloperoxidase reaction events monitored at single molecule level: Comparison between a Haloperoxidase enzyme and its inorganic biomimic<br><br><i>Gert De Cremer Universiteit Leuven</i> | 16 Integrated Plasma Catalytic Technology for Hexane Oxi-Cracking<br><br><i>Han Gardeniers TU Twente</i>   |
| 15.25          | K3<br>Supramolecular Concepts in Homogeneous Catalysis   | 7 The influence of Vanadium as dopant for La <sub>2</sub> NiO <sub>4.8</sub> in selective oxidation of propane.<br><br><i>Crapanzano S., TU Twente</i>                       | 11 Electrooxidation of adsorbed CO on stepped platinum single-crystal electrodes in alkaline media<br><br><i>Gonzalo García Leiden University</i>  | 17 Telomerization of 1,3-butadiene with polyols over a Pd/TOMPP catalytic system<br><br><i>A. N. Parvulescu University of Utrecht</i>                      |
| 15.50          | Prof. dr. Bernhard Breit - University of Freiburg, Germany   | 8 Catalytic oxi-cracking as a route to olefins<br><br><i>C. Boyadjian TU Twente</i>  | 12 In situ x-ray spectroscopy and spectromicroscopy of catalytic systems<br><br><i>Frank M.F. de Groot Universty of Utrecht Nanomaterials</i>  | 18 Chemical modification of <i>Jatropha curcas</i> oil by co-metathesis reaction<br><br><i>L. Junistia Rijksuniversiteit Groningen</i>                     |
| 16.15          | Coffee/Tea (16.15 - 16.40)<br>Poster session I: Posters with even serial numbers (Asamblea, Alegria and Oxford 22)   |  |  |  |
| 16.15          | VIRAN Membership Meeting (16.15-17.45, Cambridge 32)   |  |  |  |
| 18.15          | Dinner (18.15 - 19.45)   |  |  |  |
|                | Career Development & Opportunities   |  |  |  |
| 19.45          | CDO lecture  |  |  |  |
| 20.15          | Career Development & Opportunities Session   |  |  |  |

| Tuesday March 3, morning |   |  |   |   |
|--------------------------|---|--|---|---|
| 8.30                     | <b>P3</b> Structure Sensitivity and Insensitivity of Surface and Bulk Chemical Reactions Prof. dr. Rutger van Santen - TU/e, The Netherlands  |  |   |   |
| 9.15                     | <b>P4</b> Zeolites meet metal-organic framework materials in chemical industry Dr. Ulrich Müller - BASF Ludwigshafen, Germany   |  |   |   |
| 10.00                    | Coffee/Tea (10.00-10.30)  |  |   |   |
|                          | Rotonde   | Sorbonne 2   | Cambridge 32  | Cambridge 30  |
|                          | <i>Homogeneous Catalysis</i>  | <i>Heterogeneous Catalysis</i>   | <i>Tools: Theory, Spectroscopy and Model Catalysts</i>  | <i>(Bio)organic synthesis and catalysis</i>   |
| 10.30                    | <b>19</b><br>Effect of 6-alkyl substituted 2,2'-bipyridines in the Pd-catalyzed styrene carbonylation: shifting the selectivity from polyketones to oligoketones<br><i>D Amora, A., Università di Trieste</i> | <b>K4</b><br><br>Heterogeneously catalysed reactions in the liquid phase<br><br><br><br><br><br><br><br><br><br><b>Prof. dr. Chris Hardacre - Queens University Belfast, Ireland</b> | <b>27</b><br><br>Grafted Organotin Catalyst and Catalytic Process Monitoring Using Advanced Interface NMR<br><br><i>Rudolph Willem Vrij Universiteit Brussel</i>                          | <b>32</b><br><br>A New Regeneration System for Oxidized Nicotinamide Cofactors<br><br><i>Seda Aksu TU Delft</i>   |
| 10.55                    | <b>20</b><br><br>Towards DNA based transition metal catalysts<br><br><br><br><br><i>Ernsting, J.E, University of Amsterdam, HIMS</i>  |  | <b>28</b><br><br>Understanding automotive exhaust catalysis: Reaction and interaction between CO and NO on the surface of Rh(100)<br><br><i>Maarten M.M. Jansen TU/e Niemantsverdriet</i> | <b>33</b><br><br>Recyclable Homogeneous Dendritic Catalysts for Tandem Reactions in Semi-Permeable Compartments<br><br><i>Niels J.M. Pijnenburg University of Utrecht</i>                     |
| 11.20                    | <b>21</b><br>In search for single-component homogeneous catalysts for ethylene oligo- and polymerization: the role of the metal oxidation state<br><i>Duchateau, R. TU/e</i>                                  | <b>24</b><br><br>Platinum Nano-Particles on and in Colloidal Silica Carriers<br><br><i>Vincenzo Roberto Calderone Utrecht University</i>   | <b>29</b><br><br>How the C-C bond breaks in fuel cell ethanol oxidation<br><br><i>Steven E.F. Kleyn Leiden university</i>   | <b>34</b><br><br>DNA-based micellar catalysis<br><br><i>Fiora Rosati Rijksuniversiteit Groningen</i>  |
| 11.45                    | <b>22</b><br>Asymmetric Nickel-catalysed reductive coupling reactions of 1,3-dienes with aldehydes<br><i>Teichert, F Rijksuniversiteit Groningen</i>  | <b>25</b><br><br>Highly active CeO <sub>2</sub> -supported Au clusters for butadiene hydrogenation<br><br><i>Yejun Guan TU/e</i>   | <b>30</b><br><br>Zeolites in the act: A combined micro-spectroscopic approach<br><br><i>Marianne H.F. Kox, University of Utrecht</i>  | <b>K5</b><br><br>Recent Advances in the Combination of Metal and enzyme Catalysis--<br><br><br><br><br><br><br><br><br><br><b>Prof. dr. Jan-Erling Bäckvall- Stockholm University, Sweden</b> |
| 12.10                    | <b>23</b><br>Aromatic diselenides as catalysts in the oxidation of alcohols: the unexpected effect of substituents<br><br><i>Toorn, J.C. TU Delft</i>   | <b>26</b><br><br>On the origin of the cobalt particle size effect in Fischer-Tropsch catalysis<br><br><i>J.P. den Breejen Utrecht University</i>                                     | <b>31</b><br><br>A methodology for predictive modeling in homogeneous catalysis: applications in green chemistry<br><br><i>Ana G. Maldonado University of Amsterdam, HIMS</i>             |   |
| 12.35                    | Lunch (12.35-13.45)<br>Poster session II: Posters with odd serial numbers (Asamblea, Alegria and Oxford 22)   |  |   |   |

| Tuesday March 3, afternoon |   |   |  |  |
|----------------------------|---|---|--|--|
| 13.45                      | <b>P5 Coordination Chemistry with pi Radical Ligands: Where are the (Valence) Electrons</b> Prof. dr. Karl A. Wieghardt - Max Planck Institut fuer Bioanorganische Chemie, Muelheim a/d Ruhr, Germany |   |  |  |
|                            | Rotonde   | Sorbonne 2  | Cambridge 32   | Cambridge 30   |
|                            | <b>Homogeneous Catalysis</b>  | <b>Coordination Chemistry and Organometallic Chemistry</b>  | <b>Heterogeneous Catalysis</b>   | <b>Micro- and Mesoporous Catalytic Materials</b>   |
| 14.35                      | <b>K6</b><br><b>NMR Studies on the Supramolecular Structure of Catalytically-Important Transition-Metal Complexes</b><br><br><b>Prof. dr. Alceo Macchioni - University of Perugia, Italy</b>          | <b>36</b><br>Synthesis and Characterization Studies of a Two-Step Spin-Crossover Mononuclear Iron(II) complex with a [HS-LS-LS] Intermediate Phase<br><br><i>Bonnet, SA Leiden University</i> | <b>39</b><br>Towards an ultra-stable and zero leaching supported metal oxide catalyst for liquid oxidation reactions<br><br><i>Ilke Muylaert University of Gent</i>  | <b>42</b><br>Discontinuities in the low coverage adsorption of C1-C14 linear alkanes on Na-CHA and SAPO-34.<br><br><i>Sarah Couck Vrije Universiteit Brussel</i>             |
| 15.00                      |   | <b>37</b><br>Efficient access to complex ligands for catalysis by MCR chemistry<br><br><i>Ruijter, E. VU</i>  | <b>40</b><br>Operando Raman and ATR-FTIR Spectroscopy of Liquid Phase Heterogeneous Catalytic Processes<br><br><i>María D. Hernández-Alonso University of Delft</i>  | <b>43</b><br>Impregnation of Mesoporous Silica Studied with Differential Scanning Calorimetry<br><br><i>Tamara M. Eggenhuisen University of Utrecht</i>                      |
| 15.25                      | <b>35</b><br>Selective hydroformylation of 2,2-disubstituted alkenes using chiral diphosphites<br><br><i>Cornelissen, L.L.J.M., TU/e</i>  | <b>38</b><br>Essential Building Blocks<br><br><i>Slootweg, J.C. VU</i>  | <b>41</b><br>Synthesis of Carbon Nano Fiber (CNF) based structured catalyst support layers on fused silica and silicon substrates: model systems towards multi-phase microreactors<br><br><i>D.B. Thakur TU Twente</i> | <b>44</b><br>Synthesis and integration of diameter and chirality controlled CNTs in zeolites<br><br><i>J. Van Noyen KU Leuven</i>  |
| 15.50                      | Coffee/Tea (15.50-16.10)  |   |  |  |
|                            | Rotonde   | Sorbonne 2  | Cambridge 32   | Cambridge 30   |
|                            | <b>Industrial Catalysis and Bulk Chemicals</b>  | <b>Coordination Chemistry and Organometallic Chemistry</b>  | <b>Heterogeneous Catalysis</b>   | <b>Tools: Theory, Spectroscopy and Model Catalysts</b>   |
| 16.10                      | <b>45</b><br>A new proposed mechanism for the activation of iron-based Fischer-Tropsch catalysts based on in-situ TEM-EELS measurements<br><br><i>S. Janbroers Albemarle</i>                          | <b>46</b><br>[NiFe] Complexes as Structural and Functional Models for Hydrogenases<br><br><i>Angamuthu, R Leiden University</i>   | <b>49</b><br>Desilication of ferrierite for mesoporosity generation and improved catalyst effectiveness<br><br><i>Adriana Bonilla Sanchez Catalan Institution of Chemical Research (ICIQ-Tarragona)</i>                | <b>52</b><br>Chemical reactivity of high-silica zeolites modified with gallium: the unexpected case of anionic oligomerization of alkenes<br><br><i>Evgeny A. Pidko TU/e</i> |
| 16.35                      | <b>K7</b><br><b>Industrial Catalysis; Challenges and Opportunities</b><br><br><b>Dr. Carl Mesters - Shell Amsterdam, The Netherlands</b>  | <b>47</b><br>Tris(pyrazolyl)phosphines as versatile ligands in coordination chemistry<br><br><i>Tazelaar, C.G.J. VU</i>   | <b>50</b><br>High rates of mass transfer and reaction in rotating foam reactors<br><br><i>R. Tschentscher TU/e</i>   | <b>53</b><br>Raman spectroscopy as a versatile tool for reaction monitoring in homogeneous oxidation catalysis<br><br><i>D. Pijper Rijks Universteit Groningen</i>           |
| 17.00                      |   | <b>48</b><br>Hemilabile donor-functionalized NHCs as ligands in low-valent Palladium complexes<br><br><i>Warsink, S University of Amsterdam, HIMS</i>   | <b>51</b><br>Hairy foam: Novel catalyst support for fast mass transfer in liquid phase catalytic reactions<br><br><i>J. K. Chinthaginjala TU Twente</i>  | <b>54</b><br>Direct measurement of adsorption behaviour using a sub second liquid transient ATR microreactor<br><br><i>T.J.A.Renckens TU/e</i>                               |
| 17.30                      | NWO CW Talent workshop (Sorbonne 2)<br>Membershipmeeting KNCV-section Catalysis (Cambridge 30)  |   |  |  |
| 18.15                      | Poster session II: Posters with odd serial numbers (Asamblea, Alegria and Oxford 22)  |   |  |  |
| 20.00                      | Conference Dinner (VIRAN NCCC Award + KNCV Catalysis Award)   |   |  |  |

| Wednesday March 4, morning |  |   |   |   |
|----------------------------|--|---|---|---|
|                            | Rotonde  | Sorbonne 2  | Cambridge 32  | Cambridge 30  |
|                            | <i>Industrial Catalysis &amp; Bulk Chemicals</i>   | <i>Coordination Chemistry and Organometallic Chemistry</i>  | <i>Micro- and Mesoporous Catalytic Materials</i>  | <i>Sustainable Chemistry, Energy &amp; Devices</i>  |
| 9.15                       | 55 Deep Desulfurization of Fossil Fuels by Air in lactone solvent; the remarkable absence of a role for Catalysts<br><i>X. Xu TU Delft</i>                           | K8<br><br>Theory-Assisted Elaboration of Catalysts<br><br>Prof. dr. Pascal Le Floch - CNRS, France  | 61 Carbon nanolawn growth from cellulose, an attractive catalyst carrier<br><i>J. Hoekstra University of Utrecht</i>                        | 65 Alkylation of benzyl cyanide in a microreactor - effect of hydrodynamics on reaction rate and selectivity -<br><i>J. Jovanović TU/e</i>                                |
| 9.30                       | 56 Deactivation of the catalyst during the MTO process from a molecular modeling perspective<br><i>Karen Hemelsoet Uni Gent</i>                                      |   | 62 Amino-based Metal Organic Frameworks as stable, highly active basic catalysts<br><i>J. Gascon TU Delft</i>                               | 66 Solid acid catalysts for the conversion of trioses to lactates<br><i>Paolo P. Pescarmona Catholic University of Leuven</i>   |
|                            | <i>Homogeneous Catalysis</i>   | <i>Coordination Chemistry and Organometallic Chemistry</i>  | <i>Micro- and Mesoporous Catalytic Materials</i>  | <i>Sustainable Chemistry, Energy &amp; Devices</i>  |
| 9.55                       | 57 UREAPhos: Supramolecular Bidentate Ligands for Asymmetric Hydrogenation and Hydroformylation<br><i>Meeuwissen, J. University of Amsterdam, HIMS</i>               | 59 Phenol-pyrazole based ligands towards the design of polynuclear manganese(III) complexes<br><i>Viciano-Chumillas, M Leiden University</i>  | 63 New families of hierarchical metallosilicate zeolites by desilication<br><i>Johan C. Groen Delft Solids Solutions</i>                    | 67 Upgrading fast-pyrolysis oil:hydrodeoxygenation of sugar fraction molecules from pyrolysis oil using ru/c catalysts<br><i>J. Wildschut Rijksuniversiteit Groningen</i> |
| 10.20                      | 58 Homogeneous oxidation catalysis by proline-based manganese complexes<br><i>Moelands, M.A.H. University of Utrecht</i>   | 60 Ligand Effects in Z-Selective Linear Dimerization of Phenylacetylenes by Organo Rare Earth Compounds with Mono-anionic N <sub>4</sub> -based azepine Ligands<br><i>Ge, S Rijksuniversiteit Groningen</i> | 64 Support-Dependent Shape Selectivity for Specifically Immobilized Hoveyda-Grubbs Metathesis Catalysts<br><i>Boris Van Berlo KU Leuven</i> | 68 Promoted and supported hydrotalcites for enhanced CO <sub>2</sub> capture<br><i>N.N.A.H. Meis University of Utrecht</i>  |
| 10.45                      | Coffee/tea (10.45-11.10)   |   |   |   |
|                            | <i>Homogeneous Catalysis</i>   | <i>Coordination Chemistry and Organometallic Chemistry</i>  | <i>Micro- and Mesoporous Catalytic Materials</i>  | <i>Industrial Catalysis &amp; Bulk Chemicals</i>  |
| 11.10                      | 69 Fast and Selective Hydroaminomethylation using Xanthene-based Amino-functionalised Phosphorus Ligands<br><i>Hamers, B TU/e</i>                                    | 71 Framework Engineering of Zn(II)/4,4'-bipy Porous Coordination Polymers and Carboxylate-regulator: Synthesis, Structures and Thermal Properties<br><i>Phuengphai, P Leiden University</i>                 | 73 Quantization of pore corrugation in SBA-15 by image analysis of electron tomograms<br><i>Heiner Friedrich University of Utrecht</i>      | 75 NO <sub>x</sub> storage catalysis for ultimate pure CO <sub>2</sub> fertilization in greenhouses<br><i>Michiel Makkee TU Delft</i>                                     |
| 11.35                      | 70 METAMORPhos: Adaptive Supramolecular Ligands and the Mechanistic Consequences for Asymmetric Hydrogenation<br><i>Patureau, F.W. University of Amsterdam, HIMS</i> | 72 Coordination chemistry of polycationic phosphine ligands and their application in homogeneous catalysis<br><i>Snelders, DJM University of Utrecht</i>  | 74 Carbon-Silica composites for shape selective separations<br><i>Alexios Harkiolakis KU Leuven</i>   | 76 The preparation of commercially attractive nanocatalysts: a Pd nanocatalyst as a lead-free alternative for the Lindlar catalyst.<br><i>Peter T. Witte BASF</i>         |
| 12.00                      | Lunch (12.00-13.15)  |   |   |   |

| Wednesday March 4, afternoon |  |  |  |  |
|------------------------------|--|--|--|--|
|                              | Rotonde  | Sorbonne 2   | Cambridge 32   | Cambridge 30   |
|                              | <i>Tools: Theory, Spectroscopy and Model Catalysts</i>   | <i>(Bio)organic synthesis and catalysis</i>  | <i>Homogeneous Catalysis</i>   | <i>Micro- and Mesoporous Catalytic Materials</i>   |
| 13.15                        | <b>85</b><br><b>Co-adsorption of water with hydrogen or oxygen on Ni(111)</b><br><br><i>Shan, J Gorlaeus Laboratories Leiden Uni</i>   | <b>K9</b><br><b>Enzymes as Catalysts:<br/>New opportunities for selective oxidations</b><br><br><b>Prof. dr. Isabel Arends - TU Delft, the Netherlands</b> | <b>77</b><br><b>Mechanical catalyst activation</b><br><br><i>Sijbesma, R.P. TU/e</i>   | <b>81</b><br><b>Thiophene-based Metal-Organic Frameworks</b><br><br><i>Gerard P.M. van Klink TU Delft</i>  |
| 13.40                        | <b>86</b><br><b>Reversible Enzymatic Hydrogen Production at High Temperature</b><br><br><i>S.A. Tromp TU Delft</i>   |  | <b>78</b><br><b>Supramolecular Anchoring of Transition Metal Catalysts on Support: New Materials for “Reverse Flow Reactors”</b><br><br><i>Marras, F, University of Amsterdam, HMS</i> | <b>82</b><br><b>Introducing mesoporosity in mordenites using alkaline treatment</b><br><br><i>A.N.C. van Laak</i>                                  |
| 14.05                        | <b>K10</b><br><b>Identifying the rate limiting step and its reaction site</b>  |  | <b>79</b><br><b>Asymmetric Hydrogenation of N-Aryl Imines</b><br><br><i>Mrsic, N.M. Rijksuniversiteit Groningen</i>  | <b>83</b><br><b>The shape-selective hydrogenation of FAMES and vegetable oils</b><br><br><i>Philippaerts An KU Leuven</i>                          |
| 14.30                        | <b>Prof. dr. Ib Chorkendorff - Technical University of Denmark, Denmark</b>  | <b>88</b><br><b>Chiral Separation by Enantioselective Liquid-Liquid Extraction</b><br><br><i>Bastiaan J.V. Verkuijl Rijksuniversiteit Groningen</i>        | <b>80</b><br><b>Multimetallic Supramolecular Salen Architectures for Enhanced Cooperative Catalysis</b><br><br><i>Wezenberg, S.J. ICIQ</i>   | <b>84</b><br><b>Preparation of supported nickel oxide with tunable particle size via confinement</b><br><br><i>M. Wolters Universty of Utrecht</i> |
| 15.00                        | <b>P7</b> <b>Platinum anticancer coordination compounds: Study of DNA binding inspires new drug design</b> <b>Prof. dr. Jan Reedijk - Leiden University, The Netherlands</b> |  |  |  |
| 15.45                        | Lecture Awards, Poster Awards and Game Award - Closing (Rotonde)   |  |  |  |