

Designing New Heterogeneous Catalysts

Faraday Discussion



4-6 April 2016
London, UK

PROGRAMME

Monday 4th April

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| 11:00 | Registration, Tea and Coffee | |
| 12.00 | Lunch | |
| 12.30 | Welcome and Introductions | |
| 12.40 | Outline of Discussion Format Faraday Discussion, Publishing Editors | |
| 12.45 | Introductory Lecture (Session Chair: Graham Hutchings) Avelino Corma <i>Instituto de Tecnología Química, Spain</i> | |
| | Session 1: Designing new catalysts: synthesis of new active structures Session Chair: Jacob Moulijn | |
| 13.45 | Using degrees of rate control to improve selective <i>n</i>-butane oxidation over model MOF-encapsulated catalysts: sterically-constrained Ag₃Pd(111) <u>Charles T. Campbell</u> , Sean T. Dix, Joseph K. Scott and Rachel B. Getman <i>University of Washington, USA</i> | Paper 9133 |
| 13.50 | The cluster beam route to model catalysts and beyond <u>Richard Palmer</u> , Peter R. Ellis, Christopher M. Brown, Peter T. Bishop, Jinlong Yin, Kevin Cooke, William D. Terry, Jian Liu and Feng Yin <i>University of Birmingham, UK</i> | Paper 9577 |
| 13.55 | Active site densities, oxygen activation and adsorbed reactive oxygen in alcohol activation on npAu catalysts <u>Robert Madix</u> , C.M Friend and Lu-Cun Wang <i>Harvard University, USA</i> | Paper 9610 |
| 14.00 | Discussion | |
| 15.15 | Afternoon Tea | |
| 15.45 | Photo-spectroscopy of mixtures of catalyst particles reveals their age and type <u>Bert Weckhuysen</u> , M. M. Kersters, A. Wilbers, J. Kramer, P. de Peinder, G. Mesu, B. Nelissen and E. T. C. Vogt <i>Utrecht University, The Netherlands</i> | Paper 9138 |
| 15.50 | New crystalline complex metal oxides created by unit-synthesis and their catalysis based on porous and redox properties <u>Wataru Ueda</u> , Zhenxin Zhang, Satoshi Ishikawa, Yuta Tsuboi, Masahiro Sadakane and Toru Murayama <i>Kanagawa University, Japan</i> | Paper 9551 |
| 15.55 | Hydrothermal synthesis of bi-functional nanostructured | Paper |

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| | manganese tungstate catalysts for selective oxidation <i>Annette Trunschke, Xuan Li, Thomas Lunkenbein, Jutta Kröhnert, Verena Pfeifer, Frank Girgsdies, Frank Rosowski and Robert Schlögl</i> <i>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany</i> | 9606 |
| 16.00 | Design and stabilisation of a high area iron molybdate surface for the selective oxidation of methanol to formaldehyde <i>Peter Wells, Stephanie Chapman, Catherine Brookes, Michael Bowker, and Emma K. Gibson</i> <i>UCL, UK Catalysis Hub, RCaH, UK</i> | Paper 9483 |
| 16.05 | Discussion | |
| 17.45 | Lightning Poster Session (by invitation of the Scientific Committee) | |
| 18.00 | Poster Session (even numbers) and Wine Reception | |
| 19.15 | Close of Sessions | |

Tuesday 5th April

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| | Session 2: Catalyst design from theory to practice Session Chair: Dave Willock | |
| 09:00 | Methanol formation from CO₂ catalyzed by Fe₃S₄{111}: formate versus hydrocarboxyl pathways <i>Alberto Roldan, Nora de Leeuw</i> <i>Cardiff University, UK</i> | Paper 9134 |
| 09:05 | A unified view on heterogeneous and homogeneous catalysts through a combination of spectroscopy and quantum chemistry <i>Dimitrios Manganas, Annette Trunschke, Robert Schlögl and Frank Neese</i> <i>Max Planck Institut for Chemical Energy Conversion, Germany</i> | Paper 9514 |
| 09:10 | Quantum chemistry of the oxygen evolution reaction on cobalt(II,III) oxide – implications for designing the optimal catalyst <i>Craig Plaisance, Karsten Reutera and Rutger A. van Santen</i> <i>TU München, Germany</i> | Paper 9140 |
| 09:15 | Discussion | |
| 10.30 | Morning Tea | |
| 11.00 | Brønsted activity of two-dimensional zeolites compared to bulk materials <i>Joachim Sauer</i> <i>Humboldt-Universität zu Berlin, Germany</i> | Paper 9137 |
| 11.05 | Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts <i>Richard Catlow, , Alexander J. O'Malley, A. J. Logsdail, and A. A. Sokol</i> <i>University College London, UK</i> | Paper 9486 |
| 11:10 | The bifurcation point of the oxygen reduction reaction on Au–Pd nanoalloys <i>Jakub Staszak Jirkovský, Elisabet Ahlberg, Itai Panas and David J. Schiffrin</i> <i>University of Liverpool, UK</i> | Paper 9467 |

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| 11:15 | Discussion | |
| 12.30 | Lunch | |
| | Session 3: Bridging model and real catalysts Session Chair: Mike Bowker | |
| 13.30 | Supports and modified nano-particles for designing model catalysts <u>Hans-Joachim Freund</u> , C. P. O'Brien, K.-H. Dostert, M. Hollerer, C. Stiehler, F. Calaza, S. Schauer mann, S. Shaikhutdinov and M. Sterrer <i>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany</i> | Paper 9135 |
| 13.35 | Effects of particle size and edge structure on the electronic structure, spectroscopic features, and chemical properties of Au(111)-supported MoS₂ nanoparticles <u>Albert Bruix</u> , Jeppe V. Lauritsen and Bjørk Hammer <i>Aarhus University, Denmark</i> | Paper 9615 |
| 13.40 | High spatial resolution mapping of chemically-active self-assembled N-heterocyclic carbenes on Pt nanoparticles <u>Elad Gross</u> and Y. Levratovsky <i>The Hebrew University of Jerusalem, Israel</i> | Paper 9531 |
| 13.45 | Discussion | |
| 15.00 | Afternoon Tea | |
| 15.30 | Designing for selectivity: weak interactions and the competition for reactive sites on gold catalysts <u>Cynthia Friend</u> , R.J Madix and C.G.F Siler <i>Harvard University, USA</i> | Paper 9136 |
| 15.35 | The curious case of zeolite–clay/binder interactions and their consequences for catalyst preparation <u>Gareth Whiting</u> , Abhishek Dutta Chowdhury, Ramon Oord, Pasi Paalanen and Bert M. Weckhuysen <i>Utrecht University, The Netherlands</i> | Paper 9534 |
| 15.40 | Methanol oxidation on Fe₂O₃ catalysts and the effects of surface Mo <u>Emma Gibson</u> , M. Bowker, I. P. Silverwood and C. Brookes <i>University College London, UK</i> | Paper 9579 |
| 15.45 | Discussion | |
| 17.00 | Lightning Poster Session (by invitation of the Scientific Committee) | |
| 17.15 | Poster Session (odd numbers) and Wine Reception | |
| 18.30 | Close of Sessions | |
| 19:00 | Conference Dinner at Royal Society, 6-9 Carlton House Terrace, London | |

Wednesday 6th April

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| | Session 4: Application of novel catalysts Session Chair: Phil Landon | |
| 09.00 | The preparation of large surface area lanthanum based perovskite supports for AuPt nanoparticles: tuning the glycerol oxidation reaction pathway by switching the perovskite B site <u>Simon Kondrat</u> , Christopher D. Evans, Paul J. Smith, Troy D. Manning, Peter J. Miedziak, Gemma L. Brett, Robert D. Armstrong, Jonathan K. Bartley, Stuart H. Taylor, Matthew J. Rosseinsky and Graham J. Hutchings <i>Cardiff University, UK</i> | Paper 9139 |
| 09.05 | Selective hydrogenation of halogenated arenes using porous manganese oxide (OMS-2) and platinum supported OMS-2 catalysts <u>Haresh G Manyar</u> , Christopher Hardacre, Iain J. McManus, Helen Daly, S. F. Rebecca Taylor and Jillian M. Thompson <i>Queens University Belfast, UK</i> | Paper 9595 |
| 09.10 | The development of a new generation methyl chloride synthesis catalyst <u>David Lennon</u> , Alastair R. McInroy, John M. Winfield, Chris C. Dudman and Peter Jones <i>University of Glasgow, UK</i> | Paper 9580 |
| 09.15 | A transition metal oxofluoride offering advantages in electrocatalysis and potential use in applications <u>Henrik Svengren</u> , N. Torapava, I. Athanassiadis, S. I. Ali and M. Johnsson <i>Stockholm University, Sweden</i> | Paper 9510 |
| 09.20 | Discussion | |
| 11.00 | Morning Tea | |
| 11.30 | Acetylene hydrogenation over structured Au-Pd catalysts <u>James Anderson</u> , Alan J. McCue and Richard T. Baker <i>University of Aberdeen, UK</i> | Paper 9132 |
| 11:35 | Ammonia decomposition catalysis using lithium-calcium imide <u>Hazel Hunter</u> , Joshua W. Makepeace, Thomas J. Wood, Ronald I. Smith, Claire A. Murray and William I. F. David <i>ISIS Facility, STFC, UK</i> | Paper 9564 |
| 11:40 | Novel bifunctional catalysts based on crystalline multi-oxide matrices containing iron ions for CO₂ hydrogenation to liquid fuels and chemicals <u>Moti Herskowitz</u> , N. Utsis, R. Vidruk-Nehemya and M. V. Landau <i>Ben-Gurion University of the Negev, Israel</i> | Paper 9489 |
| 11.45 | Discussion | |
| 13.00 | Concluding Remarks (Session Chair: Robbie Burch) Bruce Gates <i>University of California, Davis, USA</i> | |
| 13.45 | Acknowledgements | |
| 14.00 | Close of meeting and lunch | |

Presenting authors are indicated in the programme by an underline. The affiliation is for the presenting author. If the presenting author of your paper has changed since abstract selection please email events@rsc.org. Please note that this is a draft programme and timings may change.