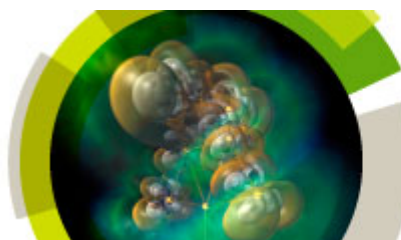


Designing New Heterogeneous Catalysts

Faraday Discussion



4-6 April 2016
London, UK

PROGRAMME

Monday 4th April

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) Charles T. Campbell, 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 Richard Palmer, 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 Robert Madix, 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 Bert Weckhuysen, 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 Wataru Ueda, 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

	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

	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 Reuter 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

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. Schauermaun, 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

	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.