

Programme

Faraday Discussion 152: Gold
4 - 6 July 2011
Cardiff University, Wales, UK

Monday 4 July

12:30	Lunch
13:30	Welcome and Introductions
Session 1	Gold Catalysis & Materials Science Session Chair: Professor Graham Hutchings, <i>Cardiff University, UK</i>
13:45 Paper 1	Introductory Lecture Masatake Haruta <i>Tokyo Metropolitan University, Japan</i>
14:45 Paper 2	Gold nanoparticle-polymer/biopolymer complexes for protein sensing Vincent Rotello*, Daniel F Moyano, Subinoy Rana and Uwe H F Bunz <i>University of Massachusetts Amherst, USA</i>
14:50 Paper 3	The active site behaviour of electrochemically synthesised gold nanomaterials Anthony P O'Mullane, Blake J Plowman and Suresh K. Bhargava* <i>RMIT University, Australia</i>
15:45	Afternoon Tea
16:15 Paper 4	Aberration corrected analytical electron microscopy studies of Sol-Immobilized Au{Pd} and Pd {Au} catalysts used for benzyl alcohol oxidation and hydrogen peroxide production R.C. Tiruvalam, J. Pritchard, N. Dimitratos, J.A. Lopez-Sanchez, J.K. Edwards, A.F. Carley G.J. Hutchings and C.J. Kiely* <i>Lehigh University, USA</i>
16:20 Paper 5	Nanoporous gold: a new gold catalyst with tunable properties Arne Wittstock*, Andre Wichmann, Jürgen Biener and Marcus Bäumer <i>University Bremen, Germany</i>
17:20	An introduction to the Poster Session Trevor Keele, <i>The World Gold Council</i>
17:30 – 19:00	Poster Session Sponsored by The World Gold Council

Tuesday 5 July

Session 2	Theoretical Insights on Gold Catalysis Session Chair: Professor Rutger van Santen, <i>Eindhoven University of Technology, The Netherlands</i>
09:00 Paper 7	New insight into the mechanism of water-gas-shift reaction on Au/CeO₂ (111): A density functional theory and kinetic study Peijun Hu*, Ying Chen, Haifeng Wang, Robbie Burch and Christopher Hardacre <i>Queens University Belfast, UK</i>
09:05 Paper 8	A periodic DFT study of the activation of O₂ by Au nanoparticles on α-Fe₂O₃ David J. Willock* and Kara L. Howard <i>Cardiff University, UK</i>
09:10 Paper 9	Free gold clusters: beyond the static, monostructure description E. C. Beret*, L. M. Ghiringhelli and M. Scheffler <i>Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin, Germany</i>
10:30	Morning Coffee
11:00 Paper 10	Aurophilic attractions between a closed-shell molecule and a gold cluster Pekka Pyykko*, Xiao-Gen Xiong and Jun Li <i>University of Helsinki, Finland</i>
11:05 Paper 11	Theoretical insights into the superior activity of gold catalysts and reactions of organogold intermediates with electrophiles A Stephen K. Hashmi*, Max Hansmann and Markus Pernpointner <i>Universität Heidelberg, Germany</i>
11:10 Paper 12	A computational investigation of H₂ adsorption and dissociation on Au nanoparticles supported on TiO₂ surface Andrey Lyalin* and Tetsuya Taketsugu <i>Hokkaido University, Japan</i>
12:30	Close of Session and Lunch/Posters

Session 3	Gold Catalysis at the Gas-Solid Interface Session Chair : Professor Mike Bowker, <i>Cardiff University, UK</i>
14:00 Paper 13	Insights into Catalysis by Gold Nanoparticles and their Support Effects through Surface Science Studies of Model Catalysts Charlie T Campbell*, James C Sharp, Y X Yao, Eric M Karp and Trent L Silbaugh <i>University of Washington, USA</i>
14:05 Paper 14	The paradigm for predicting selective oxidation on noble metals; oxidative catalytic coupling of amines and aldehydes on metallic golds Robert J Madix*, Bingjun Xu and Cynthia M Friend <i>Harvard University, USA</i>
14:10 Paper 15	Catalytic properties of supported gold nanoparticles: new insights into the size-activity relationship gained from in <i>operando</i> measurements M.-C. Saint-Leger*, I. Laoufi, A Bailly, O Robach, S. Garaudée and P Dolle <i>Institut Néel, CNRS et Université Joseph Fourier, France</i>
15:30	Afternoon Tea
16:00 Paper 16	Exploring the structure and chemical activity of 2-D gold islands on grapheme moiré/Ru (0001) Wayne Goodman, Ye Xu*, Lymarie Semidey-Flecha, Li Liu and Zihao Zhou <i>Texas A&M University, USA</i>
16:05 Paper 23	The Effect of the Metal to Non-Metal Transition on the Activity of Gold Catalysts Geoffrey Bond* <i>Brunel University, UK</i>
17:10	Close of Session
19:00	Pre-Dinner Drinks in Aberdare Hall
19:30	Conference Dinner in Aberdare Hall

Wednesday 6 July

Session 4	Gold catalysis and enhanced selectivity Session Chair: Professor Graham Hutchings, <i>Cardiff University, UK</i>
09:00 Paper 19	Oxidative coupling of alcohols on gold: insights from experiments and theory Cynthia Friend* and Bingjun Xu <i>Harvard University, USA</i>
09:05 Paper 20	Kinetic study of propylene epoxidation with H₂ and O₂ over Au/Ti-SiO₂ in the explosive region T Alexander Nijhuis*, Jiaqi Chen, Sander J A Halin and Jaap C Schouten <i>Eindhoven University of Technology, The Netherlands</i>
09:10 Paper 21	Methane activation and partial oxidation on free gold and palladium clusters: Mechanistic insights into cooperative and highly selective cluster catalysis Sandra M. Lang and Thorsten M. Bernhardt* <i>Universitat Ulm, Germany</i>
10:30	Morning Coffee
11:00 Paper 22	Gold catalyzed liquid phase oxidation of alcohol: the issue of selectivity Laura Prati*, A Villa, C E Chan-Thaw, R Arrigo, D Wang and S S su <i>Universita degli Studi di Milano, Italy</i>
11:05 Paper 26	Enhanced performance of the catalytic conversion of allyl alcohol to 3-hydroxypropionic acid using bimetallic gold catalysts Ermelinda Falletta, Cristina Della Pina*, Michele Rossi, Qian He, Christopher J. Kiely, and Graham J. Hutchings <i>Universita degli Studi di Milano, Italy</i>
11:10 Paper 24	Preparation of Ultra Low Loaded Au Catalysts for Oxidation Reactions Jennifer K Edwards*, Adrian Thomas and Qian He <i>Cardiff University, UK</i>
12:30 Paper 25	Concluding Remarks Martyn Poliakoff <i>University of Nottingham, UK</i>
13:00	Acknowledgements
13:15	Close of Meeting