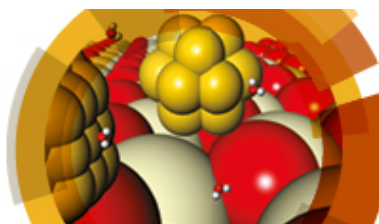


Designing Nanoparticle Systems for Catalysis



16–18 May 2018,
London, UK

Wednesday 16 May

11:30	Registration, Tea and Coffee	
12:00	Lunch	
12:45	Welcome and Introductions Graham Hutchings, <i>Chair of Scientific Committee</i>	
12:55	Outline of Discussion Format <i>Royal Society of Chemistry Publishing Editors</i>	
13:00	Introductory Lecture (Session Chair: Graham Hutchings) <u>Bruce Gates</u> <i>University of California, Davis, USA</i>	Paper 18900
	Session 1: Theory as a driving force to understand reactions on nanoparticles (Session Chair: Richard Catlow)	
14:00	The challenge of catalyst prediction <u>R. A. van Santen</u> , Aditya Sengar and Erik Steurd <i>Eindhoven University of Technology, The Netherlands</i>	Paper 18907
14:05	Modelling free and oxide-supported nanoalloy catalysts: comparison of bulk-immiscible Pd–Ir and Au–Rh systems and influence of a TiO₂ support Ilker Demiroglu, Tian-E. Fan, Z. Y. Li, Jun Yuan, Tun-Dong Liu, Laurent Piccolo and Roy L. Johnston <i>University of Birmingham, UK</i>	Paper 18908
14:10	Structural behaviour of copper chloride catalysts during the chlorination of CO to phosgene Shaoliang Guan, Philip R. Davies, Emma K. Gibson, David Lennon, Giovanni E. Rossi, John M. Winfield, June Callison, Peter P. Wells and <u>David J. Willock</u> <i>Cardiff University, UK</i>	Paper 18909
14:15	Discussion	
15:30	Afternoon tea	
16:00	Stability and mobility of supported Ni_n (n = 1–10) clusters on ZrO₂(111) and YSZ(111) surfaces: a density functional theory study Abdelaziz Cadi-Essadek, Alberto Roldan and <u>Nora H. de Leeuw</u> <i>Cardiff University, UK</i>	Paper 18906
16:05	CO adsorption and oxygen activation on group 11 nanoparticles – a combined DFT and high level CCSD(T) study about size effects and activation processes <u>Wilke Dononelli</u> and Thorsten Klüner <i>Carl-von-Ossietzky Universität Oldenburg, Germany</i>	Paper 18930
16:10	The electronic properties of Au clusters on CeO₂(110) surface with and without O-defects <u>Arunabhiram Chutia</u> , David J. Willock and C. Richard A. Catlow <i>University College London and UK Catalysis Hub, UK</i>	Paper 18934
16:15	Discussion	
17:30	Flash poster presentations (by invitation of the Scientific Committee)	

18:00	Poster Session and Wine Reception
19:30	Close of sessions

Thursday 17 May

Session 2 : The challenges of characterising nanoparticulate catalysts (Session Chair: Michael Bowker)		
09:00	Time-resolved operando studies of carbon supported Pd nanoparticles under hydrogenation reactions by X-ray diffraction and absorption Aram L. Bugaev, Oleg A. Usoltsev, Andrea Lazzarini, Kirill A. Lomachenko, Alexander A. Guda, Riccardo Pellegrini, Michele Carosso, Jenny G. Vitillo, Elena Groppo, Jeroen A. van Bokhoven, Alexander V. Soldatova and <u>Carlo Lamberti</u> <i>University of Turin, Italy</i>	Paper 18893
09:05	Insights into structure and dynamics of (Mn,Fe)O_x-promoted Rh nanoparticles Maria Dimitrakopoulou, Xing Huang, Jutta Kröhnert, Detre Teschner, Sebastian Praetz, Christopher Schlesiger, Wolfgang Malzer, Christiane Janke, Ekkehard Schwab, Frank Rosowski, Harry Kaiser, Stephan Schunk, Robert Schlögl and <u>Annette Trunschke</u> <i>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany</i>	Paper 18964
09:10	Looking for the active hydrogen species in a 5 wt% Pt/C catalyst: a challenge for inelastic neutron scattering M. Carosso, A. Lazzarini, A. Piovano, R. Pellegrini, S. Morandi, M. Manzoli, J. G. Vitillo, M. Jimenez Ruiz, C. Lamberti and <u>E. Groppo</u> <i>University of Turin, Italy</i>	Paper 18910
09:15	Discussion	
10:30	Morning Tea	
11:00	CO oxidation over supported gold nanoparticles as revealed by operando grazing incidence X-ray scattering analysis Yaroslav Odarchenko, David J. Martin, Thomas Arnold and Andrew M. Beale <i>University College London, UK</i>	Paper 18945
11:05	In situ formation of the active sites in Pd–Au bimetallic nanocatalysts for CO oxidation: NAP (near ambient pressure) XPS and MS study A. V. Bukhtiyarov, I. P. Prosvirin, A. A. Saraev, A. Yu. Klyushin, A. Knop-Gericke and <u>V. I. Bukhtiyarov</u> <i>Boriskov Institute of Catalysis, Russia</i>	Paper 18920
11:10	Correlating structural dynamics and catalytic activity of AgAu nanoparticles with ultrafast spectroscopy and all-atom molecular dynamics simulations G. F. Ferbonink, T. S. Rodrigues, D. P. dos Santos, P. H. C. Camargo, R. Q. Albuquerque and <u>R. A. Nome</u> <i>Institute of Chemistry, Brazil</i>	Paper 18921
11:15	Operando study of palladium nanoparticles inside UiO-67 MOF for catalytic hydrogenation of hydrocarbons A. L. Bugaev, Alexander A. Guda, Kirill A. Lomachenko, Elizaveta G. Kamysheva, Mikhail A. Soldatov, Gurpreet Kaur, Sigurd Øien-Ødegaard, Luca Braglia, Andrea Lazzarini, Maela Manzoli, Silvia Bordiga, Unni Olsbye, Karl P. Lillerud, Alexander V. Soldatova and Carlo Lamberti <i>Southern Federal University, Russia</i>	Paper 18966

11:20	Discussion	
13:00	Lunch	
	Session 2 continued... (Session Chair: Graham Hutchings)	
14:00	Model systems in heterogeneous catalysis: towards the design and understanding of structure and electronic properties Q. Pan, L. Li, S. Shaikhutdinov, Y. Fujimori, M. Hollerer, M. Sterrer and <u>H.-J. Freund</u> <i>Fritz-Haber-Institute of the Max-Planck Society, Germany</i>	Paper 18904
14:05	Step edge structures on the anatase TiO₂ (001) surface studied by atomic resolution TEM and STM M. Ek, I. Beinik, A. Bruix, S. Wendt, J. V. Lauritsen and <u>S. Helveg</u> <i>Haldor Topsoe, Denmark</i>	Paper 18905
14:10	Discussion	
	Session 3 : Control of catalytic nanoparticle synthesis (Session Chair: Bob Tooze)	
15:00	Gold as a modifier of metal nanoparticles: effect on structure and catalysis <u>L. Prati</u> , A. Villa, A. Jouve, A. Beck, C. Evangelisti and A. Savara <i>University of Milan, Italy</i>	Paper 18902
15:05	One pot microwave synthesis of highly stable AuPd@Pd supported core-shell nanoparticles Alexander G. R. Howe, Peter J. Miedziak, David J. Morgan, Qian He, Peter Strasser and <u>Jennifer K. Edwards</u> <i>Cardiff University, UK</i>	Paper 18903
15:10	Continuous synthesis of hollow silver–palladium nanoparticles for catalytic applications Ke-Jun Wu, Yunhu Gao and <u>Laura Torrente-Murciano</u> <i>University of Cambridge, UK</i>	Paper 18795
15:15	Discussion	
16:30	Afternoon Tea	
17:00	Supported metal nanoparticles with tailored catalytic properties through sol-immobilisation: applications for the hydrogenation of nitrophenols <u>Scott M. Rogers</u> , C. Richard A. Catlow, Diego Gianolio, Peter P. Wells and Nikolaos Dimitratos <i>University College London, UK</i>	Paper 18938
17:05	The deposition of metal nanoparticles on carbon surfaces: the role of specific functional groups B. Bowden, M. Davies, <u>P. R. Davies</u> , S. Guan, D. J. Morgan, V. Roberts and D. Wotton <i>Cardiff University, UK</i>	Paper 18875
17:10	Discussion	
18:00	Close of sessions	
18:30	Pre-Dinner Drinks, Royal Society, Carlton Terrace	
19:00	Conference Dinner, Royal Society, Carlton Terrace	

Friday 18 May

	Session 4 : Application of new nanoparticle structures as catalysts (Session Chair: Chris Hardacre)	
09:00	DFT calculation of oxygen adsorption on platinum nanoparticles: coverage and size effects <u>L. G. Verga</u> , J. Aarons, M. Sarwar, D. Thompsett, A. E. Russell and <u>C.-K. Skylaris</u> <i>University of Southampton, UK</i>	Paper 18000
09:05	Advancing semiconductor–electrocatalyst systems: application of surface transformation films and nanosphere lithography <u>Katharina Brinkert</u> , Matthias Richter, Ömer Akay, Michael Giersig, Katherine T. Fountaine and Hans-Joachim Lewerenz <i>California Institute of Technology, USA</i>	Paper 18939
09:10	Discussion	
10:00	Morning Tea	
10:30	Nanoengineering ABO₃ active sites from low-energy routes (TX100-stabilised water-in-oil microemulsions, surface segregation and surface complexation on colloidal AlOOH/sol–gel Al₂O₃ surfaces) for pollution control catalysis M. P. Worsley, P. N. Forrest, S. Roesch, C. Thatcher and <u>P. A. Sermon</u> <i>Brunel University, UK</i>	Paper 18961
10:35	Effects of heat treatment atmosphere on the structure and activity of Pt₃Sn nanoparticle electrocatalysts: a characterisation case study Haoliang Huang, Abu Bakr Ahmed Amine Nassr, Verónica Celorrio, S. F. Rebecca Taylor, Vinod Kumar Puthiyapura, Christopher Hardacre, Dan J. L. Brett and <u>Andrea E. Russell</u> <i>University of Southampton, UK</i>	Paper 18001
10:40	Discussion	
11:30	Closing Remarks (Session Chair: Graham Hutchings) <u>Cynthia Friend</u> <i>Harvard University, USA</i>	Paper 18901
12:15	Acknowledgements	
12.25	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.