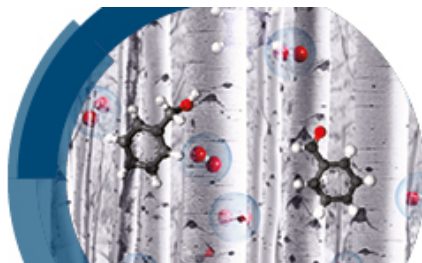


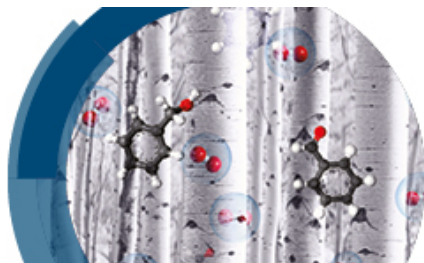
Wednesday 17 February 2021 (GMT)

11:00	Welcome and Introductions Justin Hargreaves, <i>Chair of Scientific Committee</i>
11:10	Outline of Discussion Format <i>Royal Society of Chemistry Publishing Editors</i>
11:30	Introductory Lecture (Session chair: Matthew Davidson) Graham Hutchings <i>Cardiff University, UK</i>
12:30	Break
	Session 1: Theory Session chair: Justin Hargreaves
13:00	CO₂ reduction to acetic acid on the greigite Fe₃S₄ {111} surface David Santos-Carballal, Alberto Roldan and <u>Nora H. de Leeuw</u> <i>University of Leeds, UK</i>
13:05	Addressing the uncertainty of DFT-determined hydrogenation mechanisms over coinage metal surfaces Kunran Yang and <u>Bo Yang</u> <i>ShanghaiTech University, China</i>
13:10	Structure reconstruction of metal/alloy in reaction conditions: a volcano curve? Jun Meng, <u>Beien Zhu</u> and Yi Gao <i>Chinese Academy of Sciences, China</i>
13:15	Discussion
14:15	Break
	Session 2: Theory Session chair: Justin Hargreaves
14:45	Surface stability of perovskite oxides under OER operating conditions: a first principles approach Abhinav S. Raman, Roshan Patel and <u>Aleksandra Vojvodic</u> <i>University of Pennsylvania, USA</i>
14:50	A multiscale modelling approach to elucidate the mechanism of the oxygen evolution reaction at the hematite–water interface <u>Vivek Sinha</u> , Dapeng Sun, Evert Jan Meijer, Thijs J. H. Vlugt and Anja Bieberle-Hütter <i>Dutch Institute for Fundamental Energy Research, The Netherlands</i>
14:55	A combined periodic DFT and QM/MM approach to understand the radical mechanism of the catalytic production of methanol from glycerol Mala A. Sainna, Sachin Nanavati, Constance Black, Louise Smith, Karl Mugford, Harry Jenkins, Mark Douthwaite, Nicholas F. Dummer, C. Richard A. Catlow, Graham J. Hutchings, Stuart H. Taylor, Andrew J. Logsdail and <u>David J. Willock</u> <i>Cardiff University, UK</i>
15:00	Discussion
16:00	Close of session



Thursday 18 February 2021 (GMT)

	Session 3: Advanced approaches Session chair: Jennifer Edwards / Keith Whiston
11:00	Mechanistic in situ investigation of heterogeneous hydrogenation over Rh/TiO₂ catalysts: selectivity, pairwise route and catalyst nature Ekaterina V. Pokochueva, Dudari B. Burueva, Larisa M. Kovtunova, Andrey V. Bukhtiyarov, Alexei Yu. Gladky, Kirill V. Kovtunov, Igor V. Koptug and <u>Valerii I. Bukhtiyarov</u> <i>Boreskov Institute of Catalysis, Russian Federation</i>
11:05	Effect of thermal treatment on the activity of Na-Mn-W/SiO₂ catalyst for the oxidative coupling of methane Dorota Matras, Antonios Vamvakeros, Simon D. M. Jacques, Nicolas Grosjean, Benjamin Rollins, Stephen Poulston, Gavin B. G. Stenning, Hamid R. Godini, Jakub Drnec, Robert J. Cernik and <u>Andrew M. Beale</u> <i>University College London, UK</i>
11:10	Hydrogenation of ethylene over palladium: evolution of the catalyst structure by <i>operando</i> synchrotron-based techniques <u>Aram L. Bugaev</u> , Oleg A. Usoltsev, Alexander A. Guda, Kirill A. Lomachenko, Michela Brunelli, Elena Groppo, Riccardo Pellegrini, Alexander V. Soldatov and Jeroen A. van Bokhoven <i>The Smart Materials Research Center, Southern Federal University, Russian Federation</i>
11:15	Discussion
12:15	Break
12:45	Supported Fe_xNi_y catalysts for the co-activation of CO₂ and small alkanes Shaine Raseale, Wijnand Marquart, Kai Jeske, Gonzalo Prieto, Michael Claeys and <u>Nico Fischer</u> <i>University of Cape Town, South Africa</i>
12:50	Insight into the mechanism of the water-gas shift reaction over Au/CeO₂ catalysts using <i>operando</i> spectroscopies and DFT Marc Ziemba, M. Verónica Ganduglia-Pirovano and <u>Christian Hess</u> <i>Technische Universität Darmstadt, Germany</i>
12:55	The role of oxygenated species in the catalytic self-coupling of MeOH on O pre-covered Au(111) <u>Romain Réocreux</u> , Ioanna Fampiou and Michail Stamatakis <i>University College London, UK</i>
13:00	Discussion
14:00	Break
	Session 4: Advanced approaches Session chair: Keith Whiston
14:30	Single catalyst particle diagnostics in a microreactor for performing multiphase hydrogenation reactions Anne-Eva Nieuwelink, Jeroen C. Vollenbroek, Andrea C. Ferreira de Abreu, Roald M. Tiggelaar, Albert van den Berg, Mathieu Odijk and <u>Bert M. Weckhuysen</u> <i>Utrecht University, The Netherlands</i>
14:35	Hydrogenation of substituted nitroaromatics on non-noble metal catalysts: mechanistic insights to improve selectivity Reisel Millán and <u>Mercedes Boronat</u> <i>Instituto de Tecnología Química (UPV-CSIC), Spain</i>
14:40	Combination of theoretical and <i>in situ</i> experimental investigations of the role of lithium dopant in manganese nitride: a two-stage reagent for ammonia synthesis <u>Said Laassiri</u> , Constantinos D. Zeinalipour-Yazdi, Nicolas Bion, Richard A. Catlow and Justin S. J. Hargreaves <i>University of Lille, France</i>
14:45	Discussion
15:45	Flash posters
16:15	Poster session
17:15	Close of session



Friday 19 February 2021 (GMT)

11:00	Poster session
12:00	Break
	Session 5: Advanced approaches Session chair: Keith Whiston
13:00	The interaction of CO with a copper(II) chloride oxy-chlorination catalyst Shaoliang Guan, Giovanni E. Rossi, John M. Winfield, Claire Wilson, Donald MacLaren, David J. Morgan, Philip R. Davies, David J. Willock and <u>David Lennon</u> <i>University of Glasgow, UK</i>
13:05	Reaction mechanism of low-temperature catalysis by surface protonics in an electric field <u>Yasushi Sekine</u> and Ryo Manabe <i>Waseda University, Japan</i>
13:10	Capturing spatially resolved kinetic data and coking of Ga–Pt supported catalytically active liquid metal solutions during propane dehydrogenation <i>in situ</i> <u>Moritz Wolf</u> , Narayanan Raman, Nicola Taccardi, Raimund Horn, Marco Haumann and Peter Wasserscheid <i>Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany</i>
13:15	Discussion
14:15	Break
	Session 6: Dynamics Session chair: Charlotte Williams
14:45	Multi-nuclear, high-pressure, operando FlowNMR spectroscopic study of Rh/PPh₃-catalysed hydroformylation of 1-hexene Alejandro Bara-Estaún, Catherine L. Lyall, John P. Lowe, Paul G. Pringle, Paul C. J. Kamer, Robert Franke and <u>Ulrich Hintermair</u> <i>University of Bath, UK</i>
14:50	Elucidating the role of H₂O in promoting the formation of methacrylic acid during the oxidation of methacrolein over heteropolyacid compounds <u>Sarayute Chansai</u> , Yuki Kato, Wataru Ninomiya and Christopher Hardacre <i>The University of Manchester, UK</i>
14:55	Discussion
15:35	Break
	Session 7: Dynamics Session chair: Charlotte Williams
16:05	Visualization of catalyst dynamics and development of a practical procedure to study “cocktail”-type catalytic systems Alexey S. Galushko, Evgeniy G. Gordeev, Alexey S. Kashin, Yan V. Zubavichus and <u>Valentine P. Ananikov</u> <i>Russian Academy of Sciences, Russian Federation</i>
16:10	The effect of H₂ : N₂ ratio on the NH₃ synthesis rate and on process economics over the Co₃Mo₃N catalyst Mustafa Y. Aslan, Justin S. J. Hargreaves and <u>Deniz Uner</u> <i>Middle East Technical University, Turkey</i>
16:15	Discussion
16:55	Concluding Remarks Lecture (Session Chair: Matthew Davidson) Richard Catlow <i>University College London and Cardiff University, UK</i>
17:35	Acknowledgements
17:45	Close of meeting