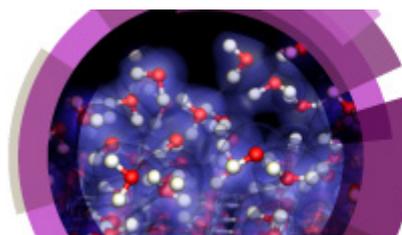


# Catalysis for Fuels

Faraday Discussion



24-26 January 2017  
Cape Town  
South Africa

**Tuesday 24 January**

11:30	Registration and Lunch	
12:45	<b>Welcome and Introductions</b> Graham Hutchings, <i>Chair of Scientific Committee</i>	
12:55	<b>Outline of Discussion Format</b> <i>Royal Society of Chemistry Publishing Editors</i>	
13:00	<b>Introductory Lecture</b> (Session Chair: Graham Hutchings) <i>Enrique Iglesia</i> <i>University of California, Berkeley</i>	
	<b>Session 1 Catalysis for Fuels</b> (Session Chair: Paul Collier)	
14:00	<b>Micro-kinetic simulations of the catalytic decomposition of hydrazine on the Cu (111) surface</b> <i>Nora de Leeuw, Tafreshi Saeedeh and Alberto Roldan</i> <i>Cardiff University, UK</i>	<b>Paper 12003</b>
14:05	<b>Theoretical insights into the sites and mechanisms for base catalyzed esterification and aldol condensation reactions over Cu</b> <i>Matt Neurock, Zhiyuan Tao, Ashwin Chemburkar, David D. Hibbitts and Enrique Iglesia</i> <i>University of Minnesota, USA</i>	<b>Paper 12004</b>
14:10	<b>Metal - support interaction on cobalt based FT catalysts – a DFT study of model inverse catalysts</b> <i>Tracey Van Heerden and Eric van Steen</i> <i>University of Cape Town, South Africa</i>	<b>Paper 12186</b>
14:15	Discussion	
15:30	Afternoon tea	
16:00	<b>Understanding FTS selectivity: the crucial role of surface hydrogen</b> <i>Kees-Jan Weststrate and J Niemantsverdriet</i> <i>SynCat@DIFFER, Syngaschem BV</i>	<b>Paper 12182</b>
16:05	<b>Computational investigation of the kinetics and mechanism of the initial steps of the Fischer-Tropsch Synthesis on cobalt</b> <i>Pieter Van Helden, Jan-Albert Van den Berg, Melissa Petersen, Werner Janse van Rensburg, Ionel Ciobica and Jan Van de Loosdrecht</i> <i>Sasol, South Africa</i>	<b>Paper 12309</b>
16:10	<b>Kinetic aspects of chain growth in Fischer–Tropsch synthesis</b> <i>Emiel Hensen, Ivo A. W. Filot, Bart Zijlstra, Robin J. P. Broos, Wei Chen and Robert Pestman</i> <i>Technische Universiteit Eindhoven, The Netherlands</i>	<b>Paper 12180</b>
16:15	Discussion	
17:30	Lightning presentations (by invitation of the scientific committee)	
17.45	Poster Session (odd numbers) and Wine Reception	
19.00	Close of sessions	

Wednesday 25 January

	<b>Session 2 Designing new catalysts for synthetic fuels</b> (Session Chair: Neil Coville)	
09:00	<b>Carbon induced selective regulation of cobalt-based Fischer-Tropsch catalysts by ethylene treatment</b> <u>Ding Ma</u> , Peng Zhai, Pei-Pei Chen, Jinglin Xie, Jin-Xun Liu, Huabo Zhao, Lili Lin, Bo Zhao, Hai-Yan Su, Qingjun Zhu and Wei-Xue Li <i>Peking University, China</i>	Paper 12006
09:05	<b>Structural and elemental influence from various MOFs on the performance of Fe@C catalysts for Fischer-Tropsch synthesis</b> <u>Freek Kapteijn</u> , Tim A. Wezendonk, Quirinus S. E. Warringa, Vera P. Santos, Adam Chojecki, Matthijs Ruitenbeek, Garry Meima, Michiel Makkee and Jorge Gascon <i>TU Delft, The Netherlands</i>	Paper 12323
09:10	<b>Size dependent stability of cobalt nanoparticles on silica under high conversion Fischer-Tropsch environment</b> <u>Michael Claeys</u> , Moritz Wolf, Hendrik Kotzé and Nico Fischer <i>University of Cape Town, South Africa</i>	Paper 12205
09:15	Discussion	
10:30	Morning Tea	
11:00	<b>Effect of crystallite size on the performance and phase transformation of Co<sub>3</sub>O<sub>4</sub>/Al<sub>2</sub>O<sub>3</sub> catalysts during CO-PrOx - an <i>in situ</i> study</b> <u>Michael Claeys</u> , Thulani Nyathi, Nico Fischer and Andrew York <i>University of Cape Town, South Africa</i>	Paper 12005
11:05	<b>The effect of sodium species on methanol synthesis and water-gas shift Cu/ZnO catalysts: utilising high purity zincian georgeite</b> <u>Simon Kondrat</u> , Paul J. Smith, James H. Carter, James S. Hayward, Geoffrey J. Pudge, Greg Shaw, Michael S. Spencer, Jonathan K. Bartley, Stuart H. Taylor and Graham J. Hutchings <i>Cardiff Catalysis Institute, UK</i>	Paper 12207
11:10	Discussion	
12:00	Lunch	
	<b>Session 2 (continued) Designing new catalysts for synthetic fuels</b> (Session Chair: Neil Coville)	
13:00	<b>PdZn catalysts for CO<sub>2</sub> hydrogenation to methanol using chemical vapour impregnation (CVI)</b> <u>Michael Bowker</u> , Hasliza Bahruji, James Hayward, Graham Hutchings, Wilm Jones, David Morgan and Jonathan Ruiz Esquius <i>Cardiff University, UK</i>	Paper 12315
13:05	<b>Selective hydrogenation of CO on Fe<sub>3</sub>S<sub>4</sub>{111}: a computational study</b> <u>Alberto Roldan</u> and Nora de Leeuw <i>Cardiff University, UK</i>	Paper 12171
13:10	<b><i>In situ</i> TEM observation of the Boudouard reaction: multi-layered graphene formation from CO on cobalt nanoparticles at atmospheric pressure</b> <u>Marien Bremmer</u> , Eirini Zacharaki, Anja Sjøstad, Violeta Navarro, Joost Frenken and Patricia Kooyman <i>Leiden University, The Netherlands</i>	Paper 12312
13:15	Discussion	
14:30	Afternoon Tea	
	<b>Session 3 Hydrocarbon conversion in the production of synthetic fuels</b> (Session Chair: Nico Fischer)	

15:00	<b>Opportunities in upgrading biomass crudes</b> <u>Avelino Corma</u> , Yannick Mattieu, Laurent Sauvanaud, Len Humphreys, Bill Rowlands and Thomas Maschmeyer <i>ITQ, Valencia, Spain</i>	<b>Paper 12008</b>
15:05	<b>Fischer-Tropsch synthesis. Evaluation of an aluminium small channel reactor</b> <u>Burtron Davis</u> , Dennis Sparks, Steven Vallee, Zhijun Jia and Wilson Shafer <i>University of Kentucky, USA</i>	<b>Paper 12204</b>
15:10	<b>Time- and space-resolved study of the methanol to hydrocarbons (MTH) reaction - influence of zeolite topology on deactivation patterns</b> <u>Unni Olsbye</u> , Daniel Rojo-Gama, Samaneh Etemadi, Eliot Kirby, Karl Lillerud, Pablo Beato and Stian Svelle <i>University of Oslo, Norway</i>	<b>Paper 12007</b>
15.15	<b>An assessment of hydrocarbon species in the methanol-to-hydrocarbon reaction over a ZSM-5 catalyst</b> <u>David Lennon</u> , S Suwardiyanto, R Howe, Emma Gibson, Richard Catlow, Ali Hameed, James McGregor, Paul Collier and Stewart Parker <i>University of Glasgow, UK</i>	<b>Paper 12011</b>
15:20	Discussion	
17:00	Lightning presentations (by invitation of the scientific committee)	
17.15	Poster Session (even numbers) and Wine Reception	
18.30	Close of sessions	
19:00	Conference Dinner	

#### Thursday 26 January

	<b>Session 4 Novel photocatalysts</b> (Session Chair: Eric Van Steen)	
09:00	<b>Particulate photocatalyst sheets for Z-scheme water splitting: advantages over powder suspension and photoelectrochemical systems and future challenges</b> <u>Kazunari Domen</u> , Qian Wang, Takashi Hisatomi, Masao Katayama, Tsuyoshi Takata, Tsutomu Minegishi, Akihiko Kudo and Taro Yamada <i>University of Tokyo, Japan</i>	<b>Paper 12009</b>
09:05	<b>Laser-flash-photolysis-spectroscopy: a nondestructive method?</b> <u>Detlef Bahnemann</u> , Jenny Schneider, Konstantin Niktin and Alexei Emeline <i>Leibniz Universität Hannover, Germany</i>	<b>Paper 12190</b>
09:10	<b>In situ spectro monitoring of CO<sub>2</sub> reduction at copper oxide electrode</b> <u>Katherine Holt</u> , Liying Wang, Kalyani Gupta, Josephine Goodall and Jawwad Darr <i>University College London, UK</i>	<b>Paper 12311</b>
09:15	Discussion	
10:30	Morning Tea	
11:00	<b>Concluding Remarks Lecture</b> (Session Chair: Hans Niemantsverdriet) Philip Gibson <i>Sasol, South Africa</i>	
11:50	<b>Acknowledgements</b>	

11:55	<b>Close of meeting and lunch</b>
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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](mailto:events@rsc.org). Please note that this is a draft programme and timings may change.