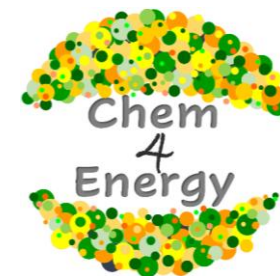


Chem4Energy Annual Conference
Materials and Processes for a Sustainable Energy Future
Monday 23 – Thursday 26 March 2026



Conference Programme (may be subject to amendment)

Monday 23 March 2026

12:30 – 13:30	<i>Lunch</i>	
13:30 – 14:00	<i>Registration</i>	<i>Albena Conference Room</i>
Session dedicated to the memory of Professor Cornie van Sittert		
14:00 – 14:10	Welcome and Opening	Professor Nora de Leeuw University of Leeds, UK; Utrecht University, The Netherlands
14:10 – 14:25	Remembering Cornie van Sittert	Professor Henning Krieg North-West University, South Africa
14:25 – 15:00	Exploring the Structure and electronic properties of ruthenium single/nanocluster adsorption on $\text{MxCe}_{1-x}\text{O}_{2-\delta}$ (111) surfaces	Dr Brian Ramogayana North-West University, South Africa
15:00 – 15:20	A beautiful life and lasting impact	Andrea Buys North-West University, South Africa
15:20 – 16:00	<i>Refreshment Break</i>	
16:00 – 16:20	DFT Analysis of NiTiO_3 and Pd-Doped NiTiO_3 Catalysts for Enhanced Photocatalytic Water Splitting	Moses Yilleng North-West University, South Africa
16:20 – 16:40	A passion for life and teaching	Cherise Thesner North-West University, South Africa
16:40 – 17:00	UK-SA Collaborations with Cornie	Professor Nora de Leeuw University of Leeds
17:00	<i>Close of session</i>	
17:30	<i>Ice Breaker drinks reception</i>	
18:30	<i>Dinner</i>	

Tuesday 24 March 2026

09:00 – 09:10	<i>Chair's comments</i>	<i>Professor Richard Catlow</i>
09:10 – 10:00	Keynote Combining DFT Modelling and Synchrotron-Based Techniques to Understand Spinel Ferrite Photocatalysts	Dr Ricardo Grau Crespo Queen Mary University of London, UK
10:00 – 10:35	Effect of TiCl _n (n = 3,4) Mediums on Ti ₁₃ Cluster	Professor Hasani Chauke University of Limpopo, South Africa
10:35 – 11:10	Au and AuCu nanoclusters for light-driven CO oxidation	Dr Igor Kowalec, Cardiff University, UK
11:10 – 11:40	<i>Refreshment break</i>	
11:40 – 12:15	Highlights of Environmental Catalytic Application of Cerium Dioxide from Density Functional Modeling	Professor Georgi N. Vayssilov University of Sofia, Bulgaria
12:15 – 12:50	Modelling Cu-based Catalysts for CO ₂ Conversion to Methanol	Dr Michael Higham Cardiff University, UK
12:50 – 14:00	<i>Lunch</i>	
14:00 – 14:10	<i>Chair's comments</i>	<i>Professor Scott Woodley</i>
14:10 – 15:00	Keynote Photocatalytic water splitting for GH ₂ production using metal oxide NPs and complexes	Professor Veikko Uahengo University of Namibia, Namibia
15:00 – 15:35	Characterization of Ir-based catalysts (Bi and tri-metal catalysts) for PEM electrolyser	Dr Shawn Gouws Nelson Mandela University, South Africa
15:35 – 16:05	<i>Refreshment Break</i>	
16:05 – 16:40	Synthesis of Zeolites from Fly Ash and their Application for Environmental Protection	Professor Yuri Kalvachev Institute of Catalysis, Bulgarian Academy of Sciences
16:40 – 17:00	The Role of Preparation Method and Surface Hydroxyl Functionality of Ordered Mesoporous Silica in Endoxylanase Immobilization	Shraddha Suman Smita Indian Institute of Technology-Madras, Indi
17:00	<i>Close of Session</i>	
18:30	<i>Dinner</i>	

Wednesday 25 March 2026

09:00 – 09:10	<i>Chair's comments</i>	<i>Professor Veikko Uahengo</i>
09:10 – 10:00	Keynote Design and preparation of functional nanomaterials, characterization and application in energy technologies	Professor Neerish Revaprasadu University of Zululand, South Africa
10:00 – 10:35	Electrically-conductive cobalt oxide thin films fabricated via the aqueous spray method using designed aqueous precursors	Dr Philipus Hishimone University of Namibia, Namibia
10:35 – 10:55	Exploring Structure-Reactivity Relationship on Plasmonically Active MOx Supported Clusters	Thomas Hill Cardiff University, UK
10:55 – 11:25	<i>Refreshment break</i>	
11:25 – 12:00	Catalytic Study of the Water-Gas Shift Reaction for Sustainable Hydrogen Production	Professor Ateeq Rahman University of Namibia, Namibia
12:00 – 12:35	In-situ large-scale catalytic H ₂ -production at near ambient P,T by molecular Fe-catalysts interfaced with inorganic particles	Professor Maria Loyludi University of Ioannina, Greece
12:35 – 14:00	<i>Lunch</i>	
14:00 – 14:10	<i>Chair's comments</i>	<i>Dr Ricardo Grau Crespo</i>
14:10 – 14:45	Is it Time to Switch to Machine Learnt Potentials?	Professor Scott Woodley University College London, UK
14:45 – 15:20	Tailoring photoresponsive azobenzene-peryene bisimide assemblies for efficient solar energy harvesting	Bongeka Ndwandwe Rhodes University, South Africa
15:20 – 15:40	Exchange-Correlation Functionals' Compatibility for the Properties of NaAlP ₂ O ₇ Solid Electrolyte Material: A DFT Study	Mamabolo Mashaole Stuart University of Limpopo, South Africa
15:40 – 16:10	<i>Refreshment Break</i>	
16:10 – 16:45	Partial Oxidation of Methanol on Gold: Microscopic Insights into Selectivity from First-Principles Simulations	Professor Lyudmila Moskaleva University of the Free State, South Africa
16:45 – 17:05	Multiscale Modelling of Hole Localisation in Cu-doped MgO and its link to Cuprate Superconductivity	Liam Morgan University College London, UK
17:05	<i>Close of Session</i>	
19:00	<i>Conference Dinner</i>	<i>The Grill Restaurant</i>

Thursday 26 March 2026

09:00 – 09:10	<i>Chair's comments</i>	<i>Professor Phuti Ngoepe</i>
09:10 – 09:45	Challenges in Computational Materials Chemistry and Physics	Professor Richard Catlow University College London and Cardiff University, UK
09:45 – 10:20	Computational Insights into the Emergence of Chirality from Achiral Bidentate Ligands	Dr George Dhimba University of Johannesburg, South Africa
10:20 – 10:55	DFT Investigation of Hydrogen Adsorption on Ti-Cluster–Decorated and N-Doped Graphene for Energy Storage Applications	Dr Tshegofatso Michael Phaahla University of Limpopo, South Africa
10:55 – 11:25	<i>Refreshment break</i>	
11:25 – 12:00	Industrial Scale Precision Engineering of H ₂ /CO ₂ Metal-Oxide Photocatalysts by Flame Spray Pyrolysis: Examples, Lessons and the TRL-Hurdles	Professor Yiannis Deligiannakis University of Ioannina, Greece
12:00 – 12:35	CO oxidation at ceria-supported few-atom gold species: role of support morphology	Dr Elena Shor Institute of Chemistry and Chemical Technology, SB Russian Academy of Sciences, Russia
12:35	Prize Giving & Closing Remarks	Nora de Leeuw University of Leeds, UK; Utrecht University, The Netherlands
12:45	<i>Close of Conference</i>	
12:45 – 14:00	<i>Lunch</i>	

Departure