

## Exploring the Viability of Utilizing Treated Wastewater as a Sustainable Water Resource for Green Hydrogen Generation Using Solid Oxide Electrolysis Cells (SOECs)

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### Introduction

The European Union aims to achieve carbon neutrality by 2050, prompting substantial investments in sustainable energy research, particularly in the realm of renewable sources (RESs). Italy, anticipating an energy demand of 366 TWh by 2030, is obligated by the EU to fulfill 75% to 84% of this demand through RESs<sup>1</sup>. A promising solution to meet this requirement is the production of green hydrogen through water electrolysis, specifically employing Solid Oxide Electrolysis Cells (SOECs). SOECs offer advantages over Alkaline Electrolyzers (AEs) and Proton Exchange Membranes (PEMs) since they can utilize treated wastewaters, eliminating the necessity for pure water, which is already scarce<sup>2,3</sup>. This study centers on exploring the potential of SOECs to operate effectively in high-temperature conditions and utilize water in its gaseous form as the inlet source, commencing with treated wastewaters derived from municipal wastewater treatment plants.

### Materials and Methods

Four distinct treated wastewaters, each characterized by differences in capacity, industrial load, and treatment scheme, underwent evaluation for their potential as feedstock in hydrogen production through Solid Oxide Electrolysis Cells (SOECs). The study employed Aspen Plus software to simulate the entire process. SOECs were spotlighted for their energy-efficient role in hydrogen production, leveraging thermal energy with a specific focus on water and air vaporization and heating. The research extensively outlined the setup of the electrolysis stack, placing emphasis on the segregation and utilization of different streams and the recuperation of residual heat from the cell products. The modeling approach for the SOEC stack encompassed equations addressing cell voltage, potential, and electric power consumption. Furthermore, the study delved into a thermal model that integrated energy and mass balance equations for various components, albeit utilizing a simplified modeling approach.

### Results and Discussion

This study illustrates that treated municipal wastewater acquired from wastewater treatment plants (WWTPs) of diverse capacities, industrial loads, and treatment schemes can function as an optimal water source for Solid Oxide Electrolysis Cells (SOECs) to generate "clean" hydrogen. Specifically, Italy is targeting the installation of 5 GW of electrolysis capacity by 2030 in alignment with the European Union's energy transition initiative. The propositions presented in this article, leveraging wastewater from various WWTPs as renewable energy sources, have the potential to aid in achieving this goal. To elaborate further, in the Best-case Scenario (BS) where a SOEC operates for 7,500 hours with a moderate power of 2.12 V supported by wind and conventional energy, a WWTP (referred to as WWTP C) with a capacity

of 120,500 P.E., an average flow rate of 27,500 m<sup>3</sup>/d, and an industrial load of 11%, can produce 0.10 Mt/y of hydrogen (equivalent to about 15% of the national target). Simultaneously, a larger WWTP (referred to as WWTP A - capacity of 620,600 P.E., average flow rate of 155,300 m<sup>3</sup>/d, and an industrial load of 15%) can generate 1.46 Mt/y, surpassing the national target. Even in the Worst-case Scenario (WS) with solely wind energy (resulting in reduced operating time to 2,000 hours per year), WWTP A remains a significant contributor, producing 0.39 Mt/y, while WWTP C contributes 0.03 Mt/y<sup>4</sup>.

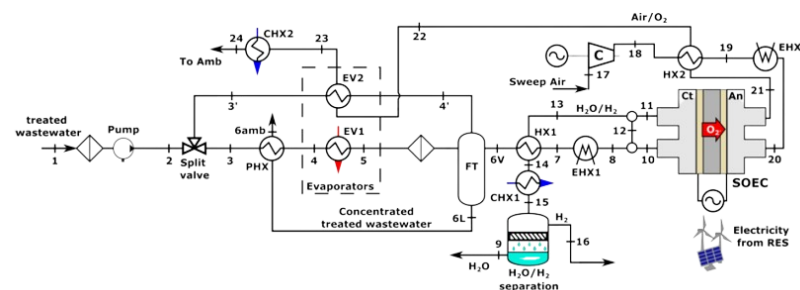


Figure 1. Layout of SOEC stack.

Converting this hydrogen production into electricity, Italy's increasing electricity demand in 2030 necessitates an annual addition of 8.6 to 10.7 GW of capacity. In the best-case scenario, WWTP A alone has the capability to fulfill 20% of the electricity demand, while in the worst-case scenario, it could cover 5.4%. For WWTP C, contributions amount to 1.3% in the best scenario and 0.4% in the worst scenario. These results underscore the considerable potential of harnessing wastewater as a sustainable and renewable energy source to address Italy's electricity requirements.

### Significance

This research illustrates that processed municipal wastewater sourced from diverse wastewater treatment facilities can serve as a superb water reservoir for Solid Oxide Electrolysis Cells (SOECs) to generate environmentally friendly hydrogen. The main objective is to emphasize the practicability and energy sustainability of utilizing wastewater as a non-potable water source for producing green hydrogen within the framework of a circular economy. This approach demonstrates efficiency in energy usage, cost-effectiveness, and holds the potential to transform the landscape of clean energy production, especially in regions with limited access to drinkable water. The amalgamation of wastewater treatment and hydrogen production has the capacity to address various sustainability objectives and contribute significantly to a decarbonized future.

### References

- 1 European Commission, *Communication from the commission to the European parliament, the council, the european economic and social committee and the committee of the regions - A European strategy for data*, 2020.
- 2 D. F. Di and L. Setti, 2022, 1–40.
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- 4 J. Arnal and M. I. Tecnalia, *H2AEOLUS-Environmental performance analysis*.



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# EXPLORING THE VIABILITY OF UTILIZING TREATED WASTEWATER AS A SUSTAINABLE WATER RESOURCE FOR GREEN HYDROGEN GENERATION USING SOLID OXIDE ELECTROLYSIS CELLS (SOECs)

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## ABSTRACT

This research addresses the European Union's pursuit of carbon neutrality by exploring the potential of water electrolysis for hydrogen production, offering a promising solution for decarbonizing existing energy systems. The **Solid Oxide Electrolysis Cell (SOEC)** is particularly attractive due to its capability to utilize impure water sources.

Using *Aspen Plus software*, this study models a **SOEC** supplied with four distinct streams of real treated municipal wastewaters of Lombardy (Italy).

Simulation analysis reveals that two wastewater streams can be efficiently evaporated and treated within the **SOEC** avoiding the generation of waste liquids with excessive pollutant concentrations.

## OBJECTIVE

- To demonstrate the possibility and energy viability of using treated municipal wastewaters obtained from real **WasteWater Treatment Plants (WWTPs)** of varying capacities, industrial loads and treatment schemes to produce “clean” hydrogen from **SOEC**.

## METHODOLOGY

- 1** Preliminary study
- 2** SOEC simulation
- 3** Data analysis
- 4** CONCLUSIONS

## RESULTS & DISCUSSION

	✓ Vaporization = 27%	Not usable. Vaporization < 10%.	✓ Vaporization = 10%	Not usable. Excessive pollutants concentration.
	WWTP A	WWTP B	WWTP C	WWTP D
Capacity [P.E.]	620,600	160,000	120,500	52,000
Average flow rate [m <sup>3</sup> /d]	155,300	50,400	27,500	23,300
Industrial load [%]	15	19	11	25
WWTP scheme	Activated sludge with pre- and post-denitrification; tertiary filtration	Membrane bioreactor (MBR) with pre-denitrification	Activated sludge with alternating oxic/anoxic cycles; tertiary filtration	Activated sludge; tertiary filtration

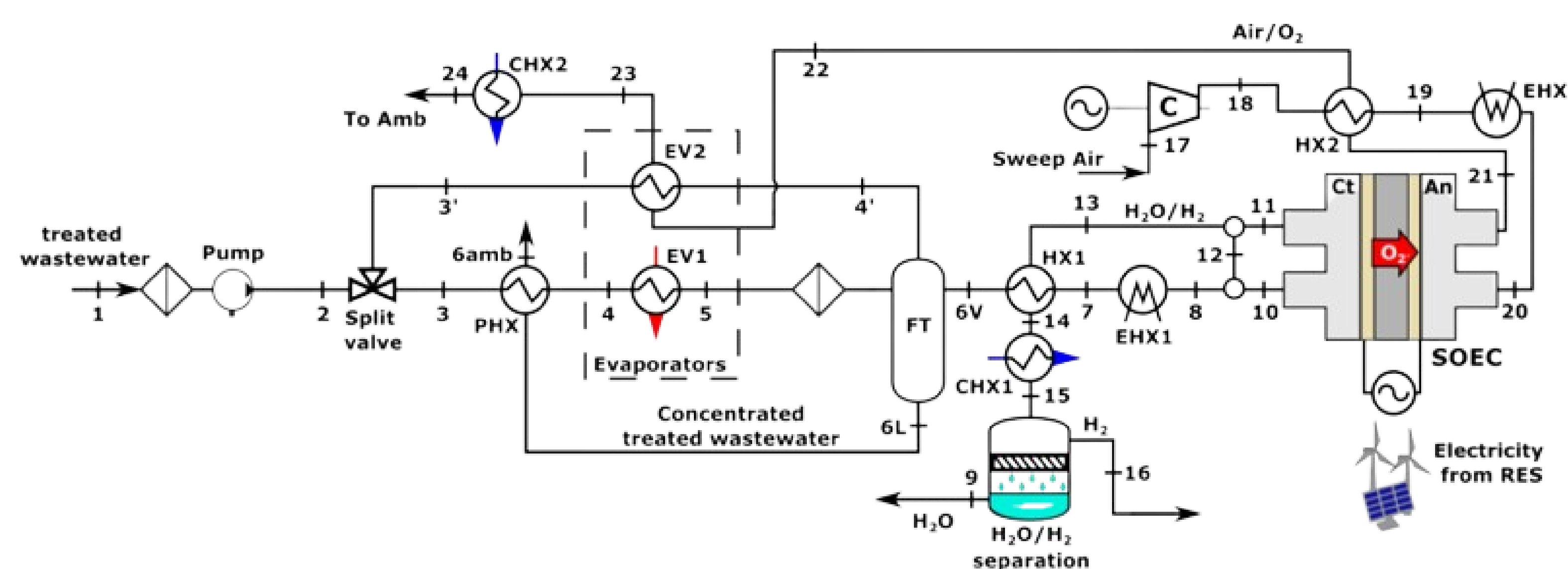
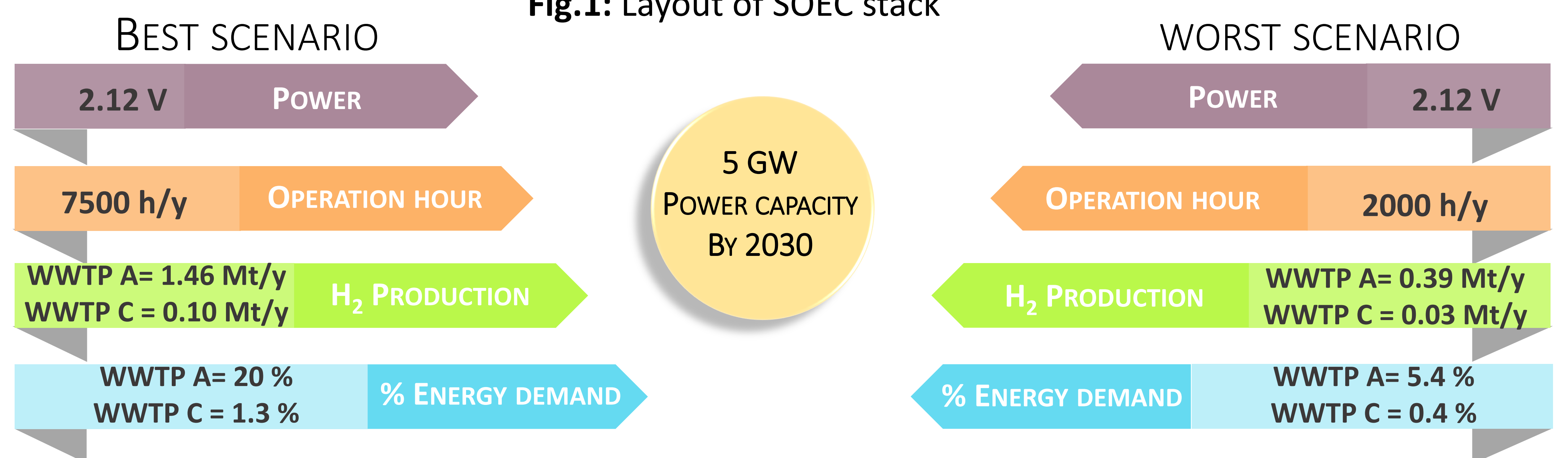


Fig.1: Layout of SOEC stack





- Two of the four wastewater streams could be effectively evaporated and treated within **SOEC**, without generating waste liquids containing excessive pollutant concentrations.
- By evaporating 27% of the first current and 10% of the second, it was estimated that 26.2 kg/m<sup>3</sup> and 9.7 kg/m<sup>3</sup> of green H<sub>2</sub> could be produced, respectively.
- Considering to have 5 GW of installed power capacity by 2030, this H<sub>2</sub> production could meet anywhere from 0.4% to 20% of Italy's projected electricity demand.



10<sup>th</sup> UK Catalysis Conference, 3-5 January 2024  
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Wednesday, 3 <sup>rd</sup> January			
11:00	Registration desk opens at Burleigh Court Hotel		
12:30	Lunch at Holywell Park		
13.50	Welcome – Conference commences at Holywell Park		
	Chair – Prof. Chris Hardacre		
14.00	PI 01 – Prof. Richard Catlow ( <i>Turing Lecture Theatre</i> )		
14.45	Coffee		
	Session A ( <i>Turing Lecture Theatre</i> )  	Session B ( <i>Brunel/Murdoch Lecture Theatre</i> )	Session C ( <i>Stephenson Lecture Theatre</i> )
<b>Chair/IT</b>	Beale/Centeno	Kondrat/Mazumdar	Garforth/Inrirai
15.15	K1 (Weller)	O4	O11
15.35		O5	O12
15.55	O1	O6	O13
16.15	O2	O7	K2 (Matam)
16.35	O3	O8	
16.55	Coffee		
<b>Chair/IT</b>	Artioli/Maddaloni	Lennon/Wilding	Wang/ Nieva De La Hidalga
17.25	K3 (Fey)	O9	O14
17.45		O10	O15
18.10	Careers Question Time – ( <i>Turing Lecture Theatre</i> )		
20.00	Dinner		



Thursday, 4 <sup>th</sup> January			
Chair – Prof. Graham Hutchings			
9.00	PI 02 – Prof. Silvia Bordiga ( <i>Turing Lecture Theatre</i> )		
	Session A ( <i>Turing Lecture Theatre</i> )	Session B ( <i>Brunel/Murdoch Lecture Theatre</i> )	Session C ( <i>Stephenson Lecture Theatre</i> )
Chair/IT	Mitchell/Olsen	Simons/Asad	Petkov/Collins
	 session		
10.00	K4 (Zhang)	O18	O28
10.20		O19	O29
10.40	O16	O20	O30
11.00	Coffee		
Chair/IT	Paterson/Ross	Matam/Mazumdar	Delarmelina/Maddaloni
11.30	K5 (Gibson)	O21	O31
11.50		O22	O32
12.10	O17	O23	O33
12.30	Lunch		
Chair – Prof. Richard Catlow			
14.00	PI 03 – RSC Award Lecture – ( <i>Turing Lecture Theatre</i> )		
14.45	Coffee		
	( <i>Turing Lecture Theatre</i> )	( <i>Brunel/Murdoch Lecture Theatre</i> )	( <i>Stephenson Lecture Theatre</i> )
Chair/IT	Mulholland/Centeno	Garforth/Mohammad	Weller/Inrirai
	 session		
15.15	K6 (Artioli)	O24	O34
15.35		O25	O35
15.55	K7 (Hermans)	O26	O36
16.15		O27	O37
16.35	Coffee		
17.00 to 19.00	Poster session		
20.00	Conference Dinner		



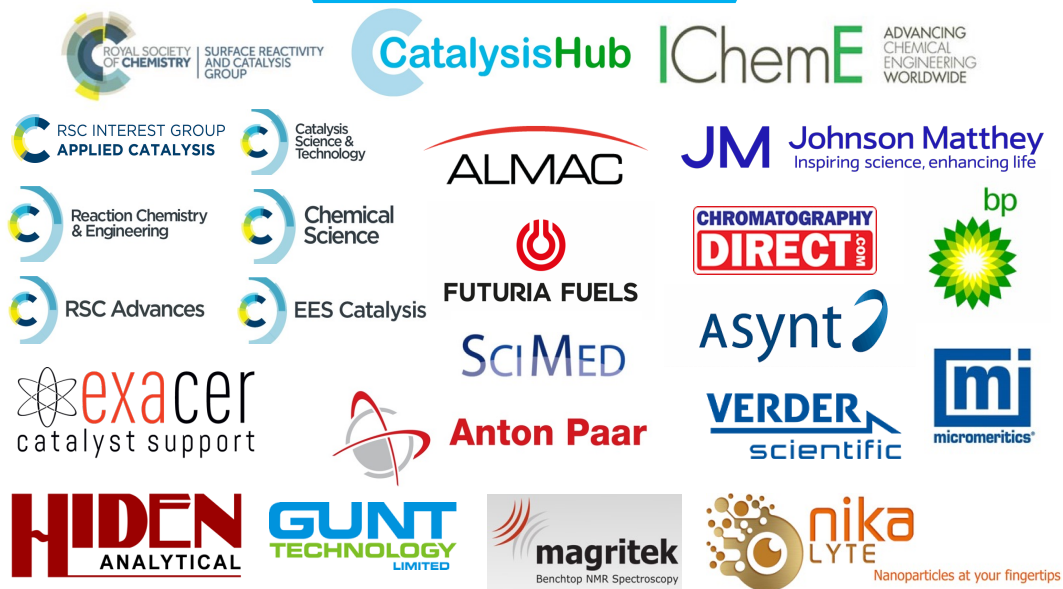
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Friday, 5 <sup>th</sup> January			
	<i>Session A (Turing Lecture Theatre)</i>	<i>Session B (Brunel/Murdoch Lecture Theatre)</i>	<i>Session C (Stephenson Lecture Theatre)</i>
<b>Chair/IT</b>	Freakley/Centeno	Zhang/Mohammad	Lin/Olsen
9.00	K8 (Nastase)	O40	O46
9.20		O41	O47
9.40	O38	O42	O48
10.00	Coffee		
<b>Chair/IT</b>	Dingwall/Ross	Fey/Asad	D'Agostino/Collins
10.30	K9 (Wang)	O43	O49
10.50		O44	O50
11.10	O39	O45	O51
	Chair – Prof. Matthew Davidson		
11.35	PI 04 – Prof. Walter Leitner ( <i>Turing Lecture Theatre</i> )		
12.20	Closing remarks		



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## PLENARY SPEAKERS



### Prof. Walter Leitner

Max Planck Institute for Chemical Energy Conversion, Germany

*New Carbon Sources for the Energetic and Chemical Value Chain: Challenges and Opportunities for Catalysis - TEN YEARS AFTER!*



### Prof. Sir Richard Catlow

Cardiff Catalysis Institute, UK

*Modelling of Catalytic Structures and Mechanisms: Achievements and Challenges*



### Prof. Silvia Bordiga

University of Turin, Italy

*MOFs and MOFs derivatives used as catalysts*

## KEYNOTE SPEAKERS

Dr. Nancy Artioli, University of Brescia, Italy and Queen's University Belfast, UK

Dr. Natalie Fey, University of Bristol, UK

Dr. Emma Gibson, University of Glasgow, UK

Prof. Ivo Hermans, University of Wisconsin-Madison, USA

Dr. Santhosh Matam, Cardiff University, UK

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## List of Talks UKCC 2024

#	Title	Authors
PI 01	Modelling of Catalytic Structures and Mechanisms: Achievements and Challenges	Richard Catlow
PI 02	MOFs and MOFs derivatives used as catalysts	Silvia Bordiga
PI 03	Innovation in Fischer-Tropsch Catalysis for an Applied Process	James Paterson
PI 04	New Carbon Sources for the Energetic and Chemical Value Chain: Challenges and Opportunities for Catalysis - TEN YEARS AFTER!	Walter Leitner
K 01	"Solid-State Molecular Organometallic Catalysis: Crystalline Molecular Factories"	Andrew Weller
K 02	Electrochemical CO <sub>2</sub> reduction over Cu-based gas diffusing electrodes: a study by complementary spectroscopic techniques	Santhosh Matam
K 03	Towards Data-Led Prediction in Homogeneous Catalysis	Natalie Fey
K 04	Mechanistic insights into the role of bi-functional and bi-metallic catalysts during hydrodeoxygenation of converting wastes into fuels	Xiaolei Zhang
K 05	The Impact of Aging on the Structure-Activity Relationships of TWC Catalysts	Emma Gibson
K 06	Novel synthesis approaches for CO <sub>2</sub> Hydrogenation catalysts using Ionic Liquids	Nancy Artioli
K 07	Understanding Surface Reactions using Modulation Excitation Spectroscopy	Ive Hermans
K 08	Methanol activation on Brønsted acid and defect sites in zeolites	Stefan Nastase
K 09	Heterogeneous catalysis mediated cofactor regeneration for biosynthesis	Xiaodong Wang
O 01	Operando X-ray photoelectron spectroscopy at the solid-liquid interface	Charalampos Drivas, Elizabeth Jones, Robert Weatherup, Mark Isaacs and Christopher Parlett
O 02	A Biocatalytic Approach Towards Alcohol Oxidation	Simon D. Anderson, Gavin J. Miller, Sebastian C. Cosgrove
O 03	Influence of Sulfation on Activity & Stability of Metal oxide Catalysts for Vapor-phase Ketonisation of Volatile Fatty Acids	Ander Centeno, Gunjan Deshmukh, Maicon Delarmelina, Helen Daly,



		Alexandre Goguet, Chris Hardacre, Richard Catlow, Haresh Manyar
O 04	Glucose isomerisation in zeolite Y: Adsorption effects on catalytic performances studied by NMR relaxation and in-situ DRIFTS	Carmine D'Agostino, Luke Forster, Mohamed M.M. Kashbor, James Railton, Sarayute Chansai, Christopher Hardacre and Marco Conte
O 05	The Origins of High Selectivity Aniline Synthesis Catalysis with Pd/Al <sub>2</sub> O <sub>3</sub> : An In Situ Infrared Spectroscopic Study	Annelouise McCullagh, Stewart Parker and David Lennon
O 06	Laser Induced Temperature-Jump Time-Resolved IR Spectroscopy of Zeolites from Nanoseconds to Seconds	Alexander P. Hawkins, Amy E. Edmeades, Christopher D.M. Hutchison, Michael Towrie, Russell F. Howe, Gregory M. Greetham and Paul M. Donaldson
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O 08	Operando characterisation of the products of Fischer-Tropsch synthesis within catalyst pellets using magnetic resonance	Qingyuan Zheng, Jack Williams, Mick Mantle, Andrew Sederman, G. Bezemer, Constant Guédon and Lynn Gladden
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P05	An investigation into the adsorption mechanism of n-butanol by ZIF-8: a combined experimental and ab initio molecular dynamics approach	Samuel Wallbridge, Stuart Archer, Jonathan Wagner, Jamieson Christie and Sandra Dann
P06	Designing Catalytic Pyrolysis of Biomass for Green Hydrogen Production	Sara Golenarges, Khalid Aziz, Johan Jacquemin, Christopher Hardacre and Marta Falkowska
P07	Hierarchically grown CeO <sub>2</sub> /GO on nylon filter with enhanced hydrophilicity and permeation flux for oil-water separation	Naseer Ahmad, Dr. Dilshad Hussain and Muhammad Ikram Nabeel
P08	Catalytic fast pyrolysis of levoglucosan, furfural and furan over HZSM-5: An experimental and theoretical investigation	Amin Osatiashtiani, Jiajun Zhang, Stylianos Stefanidis, Anthony Bridgwater and Xiaolei Zhang
P09	The Continuous Flow Synthesis of Jasminaldehyde	Ander Centeno-Pedrazo, Harry Patterson, Meabh McAtamney, Nayan Mazumdar, Dipti Wagh, Nancy Artioli, Haresh Manyar
P10	Insights into Mechanochemical Synthesis of Copper on Manganese Oxide Catalysts for Levulinic acid Hydrogenation	Nayan Jyoti Mazumdar, Praveen Kumar, Miryam Arredondo-Arechavala, Nancy Artioli, Haresh Manyar
P11	Direct Capture and Conversion of CO <sub>2</sub> to Glycerol Carbonate using CaO-CeO <sub>2</sub> Dual Function Materials in Continuous Flow	Patcharaporn Inrirai, Dipti Wagh, Gunjan Deshmukh, Nancy Artioli, Haresh Manyar
P12	"Exploring the Viability of Utilizing Treated Wastewater as a Sustainable Water Resource for Green Hydrogen Generation	Marina Maddaloni, Matteo Marchionni, Alessandro Abbá, Michele Mascia, Vittorio Tola, Maria Paola Carpanese, Giorgio Bertanza and Nancy Artioli
P13	The application of molecular spectroscopy and neutron scattering to investigate biocatalytic transamination intermediates	Ramandeep Singh Dosanjh, David Lennon and Stewart Parker

P14	Towards Avoidance of a Hydrogenolysis Step in the Liquid Phase Heterogeneously Catalysed Hydrogenation of Benzaldehyde	Asma Nadia, Colin Brennan and David Lennon
P15	Catalytic Upcycling of Low-Density Polyethylene (LDPE) using Nickel Tungstated Zirconia Catalyst	Edidiong Asuquo, Nasser Alqahtani, Hassan Alhassawi, Wenxi Zheng, Hubertus Warsahartana, Dave Scapens, Christopher Parlett and Arthur Garforth
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P18	Surface modification of TiO <sub>2</sub> with gold and copper nanoparticles for enhancing the photocatalytic H <sub>2</sub> production	Juan Medina, Agileo Hernandez-Gordillo, Sandra Rodil and Jennifer Edwards
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P22	Continuous flow enzymatic processes – controlling mass transfer with the external agitation	Nikolay Cherkasov, Daniel Lambden, Samuel Adams
P23	Using Accelerated Deactivation to Bridge the Time Gap Between Lab Testing and Long-Term Industrial Operation: A Case Study in Methanol Synthesis	Graham Lightfoot, Monica Garcia-Dieguez and Michael Nicholson
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P27	On the Order of (Mo <sub>2</sub> /3Sc <sub>1/3</sub> ) <sub>2</sub> C i-MXene Monolayer: An Ab Initio Study	Xiangchao Meng, Ryan Wang
P28	Understanding molecular behaviour in microporous catalysts for sustainable carbon conversions	Alexander O'Malley
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