HYDRO OXY

Accelerating Green Chemistry

Sustainable Routes to Global Chemicals

Cardiff University
Prifysgol Caerdydd

Cardiff Catalysis Institute
Sefydliad Catalysis Caerdydd

hydro-oxy.com

The Role of Hydrogen Peroxide in Chemical Manufacturing

Every year, nearly 2.5 million tons of hydrogen peroxide (H_2O_2) is used in chemical manufacturing. Among its most significant applications are:

- The epoxidation of propylene to propylene oxide
- The ammoximation of cyclohexanone, to cyclohexanone oxime, a key step in producing the Nylon-6 monomer, ε-caprolactam

In both cases, the utilisation of preformed H_2O_2 has presented significant improvements compared to alternative technologies including;

Lower energy inputs

Reduced purification costs

Improved atom efficiency

However, further improvements are required if the chemical sector is to reach its declared sustainability goals.

Interest has also grown in using H_2O_2 for producing other bulk chemicals, such as:

- Adipic acid
- Cyclohexanone
- Cyclohexanol
- Phenol
- Methanol

But commercialisation has been prevented due to the expense of preformed H_2O_2.

Challenges of Preformed Hydrogen Peroxide

Despite its benefits, the use of preformed H_2O_2 is limited by:

- High production costs: The cost of preformed H_2O_2 relative to the desired product inhibits commercialization in many processes.

- Environmental drawbacks: These include high water and energy consumption and significant CO_2 emissions.

- Process safety concerns associated with the storage of concentrated H_2O_2 on-site.

- Decreased reactor longevity and increased expense associated with the stabilising agents present in the preformed H_2O_2.

The Promise of in-situ H_2O_2 Production

The application of in-situ generated H_2O_2 has long been recognised as a transformative opportunity for feedstock valorisation, offering:

- Significant process intensification by decoupling chemical synthesis from industrial H_2O_2 production
- Considerable cost savings over preformed H_2O_2
- Superior environmental credentials, improving the viability of current industrial processes and opening new pathways for commodity chemical synthesis

However, earlier efforts to implement in-situ H_2O_2 production faced challenges such as:

- Low conversion rates
- Poor selectivity for desired products
- Competitive hydrogenation reactions reducing process efficiency
- Rapid catalyst deactivation

Significant process intensification

Considerable cost savings

Superior environmental credentials

Our Innovation

Building on over 20 years of research, which has led to the development of several state-of-the-art catalysts for the direction synthesis of H_2O_2. The Cardiff Catalysis Institute has recently developed a catalytic approach to cyclohexanone oxime production via in-situ H_2O_2 production.

Key features of our technology include:

- Comparable performance metrics to current industrial technology (99% yield)
- Near 100% selective utilisation of H_2
- Compatible with existing reactor infrastructure
- Decoupling of oxime production from industrial routes to H_2O_2

Techno-economic and Environmental Impact

A detailed techno-economic analysis reveals:

15% Material cost reduction

Significant environmental benefits, avoiding the need for:

Over 60 million tons of water annually

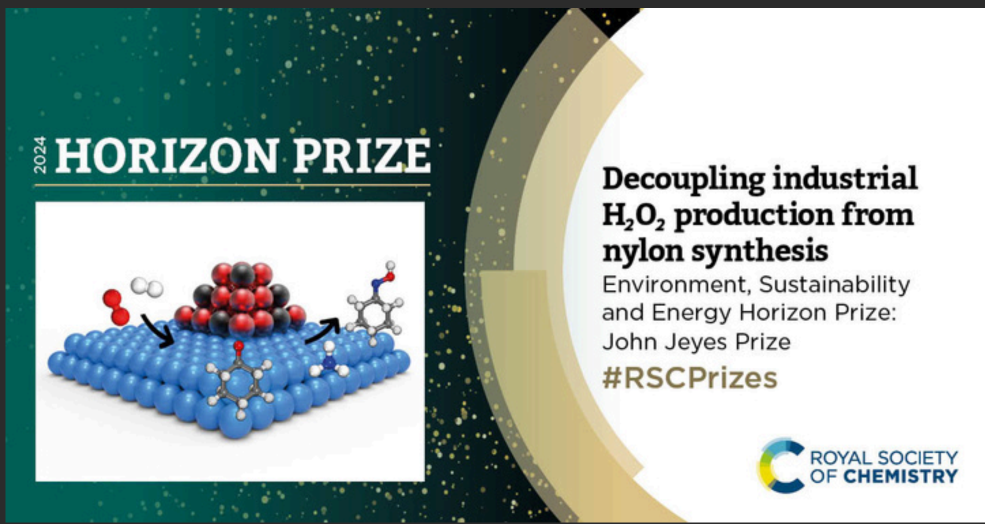
2.1 million tons of CO_2 associated with preformed H_2O_2 use in oxime production

hydro-oxy.com

Recognition and Achievements

Our innovative technology has been recognised by leading institutions and voices in the field, including:

- The Royal Society of Chemistry 2024 Environment, Sustainability and Energy Horizon Prize: John Jeyes Prize
- The Institution of Chemical Engineers, Global Awards
- Acclaim from academic and industrial leaders in leading scientific journals



Future Directions

Building on this success, the Cardiff Catalysis Institute is focusing on:

1. Commercialising the in-situ technology for cyclohexanone oxime production
2. Expanding the technologies application to the production of other commodity chemicals

HYDRO OXY

Accelerating Green Chemistry

Get In Touch

Dr. Richard Lewis

Cardiff Catalysis Institute, Cardiff University

📧 lewisr27@cardiff.ac.uk

🌐 hydro-oxy.com

CARDIFF UNIVERSITY PRIFYSGOL CAERDYDD

Cardiff Catalysis Institute

Sefydliad Catalysis Caerdydd

References

1. Edwards et al., Switching Off Hydrogen Peroxide Hydrogenation in the Direct Synthesis Process, Science, 323, 5917, 1037-1041, 2009, (10.1126/science.1168980).

2. Freakley et al., Palladium-tin catalysts for the direct synthesis of H2O2 with high selectivity, Science, 351, 6276, 965-968, 2016, (10.1126/science.aad5705).

3. Lewis et al., Highly efficient catalytic production of oximes from ketones using in situ–generated H_2O_2, Science, 376, 6593, 615-620, 2022 (10.1126/science.abl4822).

4. Lewis et al., Selective Ammoximation of Ketones via In Situ H_2O_2 Synthesis, ACS Catal., 13, 3, 1934-1945, 2023 (doi.org/10.1021/acscatal.2c05799).

5. Lewis et al., Cyclohexanone ammoximation via in situ H_2O_2 production using TS-1 supported catalysts, Green Chem., 24, 9496-9507, 2022, (doi.org/10.1039/D2GC02689A).

6. A Greener Route to Nylon Production, Winner: 2024 Environment, Sustainability and Energy Horizon Prize: John Jeyes Prize, Royal Society of Chemistry (A Greener Route to Nylon Production - 2024 Environment, Sustainability and Energy Horizon Prize: John Jeyes Prize winner).

7. IChemE celebrates 2023 Global Awards winners (IChemE celebrates 2023 Global Awards winners - IChemE).

8. Lu and Fang., Does in-situ-genertated H_2O_2 promote important industrial reactions? Chem., 8, 6, 1548-1550, 2022, (10.1016/j.chempr.2022.05.006)

9. Qiao et al., Chemical and Engineering Bases for Green H_2O_2 Production and Related Oxidation and Ammoximation of Olefins and Analogues., Natl. Sci. Rev., 11, 8, 2024, (doi.org/10.1093/nsr/nwae243).

10. Zhang et al. Recent Progress in in-situ Application of H_2O_2 produced via Catalytic Synthesis, e202402767, 2024 (doi.org/10.1002/chem.202402767).

11. Sharp et al., Benzyl Alcohol Valorisation via the In Situ Production of Reactive Oxygen Species, ACS Catal., 14, 20, 15279-15293, 2024, (doi.org/10.1021/acscatal.4c04698).

12. Crombie et al., Enhanced Selective Oxidation of Benzyl Alcohol via In Situ H_2O_2 Production over Supported Pd-Based Catalysts, ACS Catal., 11, 5, 2701-2714, 2021 (doi.org/10.1021/acscatal.0c04586).

13. Carter et al., The selective oxidation of methane to methanol using in situ generated H_2O_2 over palladium-based bimetallic catalysts, Catal. Sci. Technol., 13, 5848-5858, 2023 (doi.org/10.1039/D3CY00116D).

14. Lewis and Hutchings, Selective Oxidation Using In Situ-Generated Hydrogen Peroxide, Acc. Chem. Res., 57, 1, 106-119, 2024 (doi.org/10.1021/acs.accounts.3c00581)