Scientists discover greener route to widely used industrial material

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Scientists from Cardiff University have taken a step towards a greener, more sustainable way of creating a plastic material found in a range of items from toothbrushes and guitar strings to medical implants,

construction materials and car parts.

In a new paper published today in the journal *Science*, the team report a brand-new method of creating cyclohexanone oxime—a pre-cursor to the plastic material Nylon-6, which is a key construction material used in the automotive, aircraft, electronic, clothing and medical industries.

It is estimated that global production of Nylon-6 is expected to reach around 9 million metric tons a year by 2024, prompting scientists to search for greener and more sustainable ways of producing cyclohexanone oxime.

Currently, cyclohexanone oxime is produced industrially through a process involving hydrogen peroxide (H_2O_2), ammonia (NH_3) and a catalyst called titanosilicate-1 (TS-1).

The H_2O_2 used in this chemical process, as well as many others, is produced elsewhere and needs to be shipped in before it can be used in the chemical reaction.

This is a costly and carbon-intensive process that also necessitates the shipping of highly concentrated H_2O_2 to the end-user prior to dilution, which effectively wastes the large amounts of energy used during concentration.

Similarly, the stabilizing agents often used to increase the shelf-life of H_2O_2 can limit reactor lifetime and often they need to be removed before arriving at a final product, leading to further economic and environmental costs.

To address this issue, the team has devised a method where H_2O_2 is synthesized in-situ from dilute streams of hydrogen and oxygen, using a catalyst consisting of gold-palladium (AuPd) nanoparticles that are either

directly loaded on to the TS-1 or on a secondary carrier.

Nanoparticles, which measure roughly between 1 to 100 nanometers, are extremely useful materials to use as catalysts due to their large surface area-to-volume ratio compared to bulk materials.

The method was performed in conditions previously thought to be extremely detrimental to H_2O_2 production and can produce yields of cyclohexanone oxime comparable to those seen in current commercial processes, while avoiding the major drawbacks associated with commercial H_2O_2.

Furthermore, the team were able to demonstrate the versatility of this approach by producing a range of other industrially important chemicals, which themselves have wide ranging applications.

Lead author of the study Dr. Richard Lewis, from the Max Planck–Cardiff Center on the Fundamentals of Heterogeneous Catalysis, based at the Cardiff Catalysis Institute, said: "This work represents a positive first step towards more sustainable selective chemical transformations and has the potential to supersede the current industrial route to cyclohexanone oxime.

"The generation of H_2O_2 through this new approach could be used in a wide-range of other industrial applications that are currently dependent on the use of TS-1 and H_2O_2, potentially representing a sea change in industrial oxidation chemistry.

"This is a clear demonstration that through academic and industrial collaboration, significant improvements on current state-of-the-art technologies can be made, leading to significant cost savings and a reduction in greenhouse gas emissions from a major industrial process."

More information: Richard J. Lewis et al, Highly efficient catalytic production of oximes from ketones using in situ–generated H_2O_2, *Science* (2022). DOI: 10.1126/science.abl4822

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