Researchers work to reduce the amount of precious metals in catalytic converters

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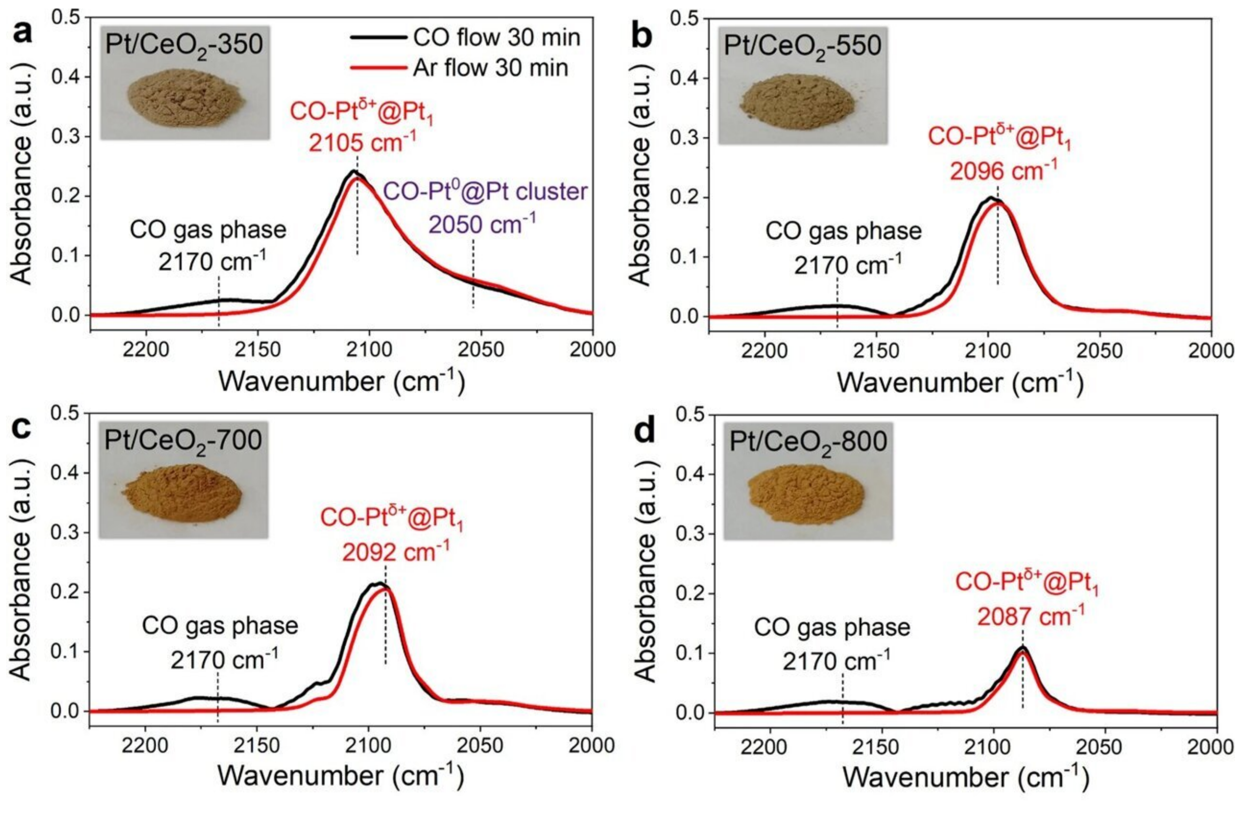

Pt status determined by CO adsorption and corresponding CO oxidation activity. Credit: *Nature Communications* (2022). DOI: 10.1038/s41467-022-34797-2

The precious metals, such as platinum, palladium and rhodium, in catalytic converters make the vehicle devices attractive to thieves, but

University of Central Florida researchers are working to reduce the amount of precious metals needed in them—down to single atoms—while still maximizing their effectiveness.

Catalytic converters, which were widely introduced in American vehicles in the 1970s, use precious metals as catalysts to help scrub deadly and harmful chemicals from combustion engine exhaust. As the price of precious metals has continued to rise, so has the number of catalytic converter thefts.

In recent studies appearing in *Nature Communications* and the *Journal of the American Chemical Society*, UCF researchers showed that they could, respectively, use atomic platinum to control pollutants and operate the system at lower temperatures, which is crucial to removing harmful chemicals when a vehicle first starts.

Fine-tuning platinum atom location

In the *Nature Communications* study, UCF research teams led by Fudong Liu, assistant professor in the Department of Civil, Environmental and Construction Engineering, and Talat Rahman, distinguished Pegasus Professor in the Department of Physics, successfully constructed platinum single atoms with different atomic coordination environments at specific locations on ceria. Ceria is a metal oxide that helps improve catalytic reaction performance.

The platinum atoms exhibited strikingly distinct behaviors in catalytic reactions, such as carbon monoxide oxidation and ammonia oxidation in a diesel engine exhaust aftertreatment system, the researchers say.

The oxidation converts deadly carbon monoxide to carbon dioxide, and harmful ammonia to nitrogen and water molecules.

Their results suggest that the catalytic performance of single atom catalysts in targeted reactions can be maximized by optimizing their local coordination structures through simple and industrial-scalable strategies, Liu says.

"By combining electronic structure calculations with state-of-the-art experiments, the Liu and Rahman teams have made a breakthrough that can significantly benefit the heterogenous catalysis community in designing highly efficient single atom catalysts for both environmental and energy related needs," Liu says.

"We have successfully developed a facile strategy to selectively fine-tune the local coordination environment of platinum single atoms to achieve satisfactory catalytic performance in different target reactions, which will push the understanding of single-atom catalysis a significant step forward," he says.

Rahman says their collaborative work demonstrates how theory and experiments working in tandem can unveil microscopic mechanisms responsible for enhancing catalytic activity and selectivity.

Efficient carbon monoxide oxidation catalyst

In the *Journal of the American Chemical Society* study, Liu and collaborators from Virginia Tech and Beijing University of Technology significantly improved the carbon monoxide purification efficiency of a platinum-ceria-alumina catalyst by 3.5 to 70 times compared to the regularly used platinum catalysts.

They did this through the precise control of coordination structures of platinum at the atomic level on an industrial-available ceria-alumina support.

"The local structure of the active site within a catalyst determines its catalytic performance," Liu says. "However, the precise control of the local coordination structure of active sites and the elucidation of intrinsic structure-performance relationships are of great challenges in the heterogeneous catalysis field."

"We've worked to control the local coordination structure of metal sites at an atomic level, develop a highly efficient catalyst in environmental purification related reactions and reveal the structure-performance relationship of the newly fabricated catalysts for guiding the future catalyst design," he says.

Using a surface defect enrichment strategy, Liu and his team reported the successful fabrication of platinum atomic single-layer and platinum single-atom structures with precisely controlled local coordination environment on ceria-alumina supports.

Using high-angle annular dark-field scanning transmission electron microscopy, one of the key co-authors, Yue Lu from Beijing University of Technology, directly observed that the platinum atomic single-layer and platinum single-atom structures showing 100% metal exposure were embedded into ceria lattice or adsorbed on ceria surface.

The embedded platinum atomic single-layer site showed the highest efficiency in carbon monoxide purification, which was 3.5 times of that on the adsorbed platinum atomic single-layer and 10 to 70 times of that on platinum single-atom sites.

In collaboration with Hongliang Xin's research group at Virginia Tech, from both experimental and theoretical aspects, the team concluded that the unique embedded platinum atomic single-layer structure could promote the activation of interfacial oxygen species and thus benefit the carbon monoxide oxidation at low temperatures.

The work is highly important because it will help the environmental catalysis community better design more active metal catalysts with 100% metal utilization efficiency for targeted environmental applications, Liu says.

"We showed how to control and utilize the structures of metal single-atom, atomic single-layer and cluster sites in emission control related reactions, and how to understand their structure-performance relationship using both experimental and theoretical simulation approaches," Liu says. "This will pave the way for future environmental catalyst design at the atomic level and achieve high efficiency in practical applications."

More information: Wei Tan et al, Fine-tuned local coordination environment of Pt single atoms on ceria controls catalytic reactivity, *Nature Communications* (2022). DOI: 10.1038/s41467-022-34797-2

Shaohua Xie et al, Pt Atomic Single-Layer Catalyst Embedded in Defect-Enriched Ceria for Efficient CO Oxidation, *Journal of the American Chemical Society* (2022). DOI: 10.1021/jacs.2c08902

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