How the catalytic converters in cars go bad and why it matters

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Modern cars rely on catalytic converters to remove carbon monoxide, hydrocarbons and other harmful chemicals from exhaust emissions.

To do so they rely on costly metals that have special chemical properties that diminish in effectiveness over time. Assistant professor Matteo Cargnello and doctoral candidate Emmett Goodman recently led a team that has proposed a new way to reduce the cost and extend the lifespan of these materials, solving a problem that has vexed automotive engineers for years. In the process, Cargnello and colleagues have done something remarkable: made a breakthrough in a mature field where change comes slowly, if at all.

What about catalytic converters needs to be improved?

A new catalytic converter can cost $1,000 or more, making it among the most expensive individual parts on any car. They are costly because they use expensive metals such as palladium to promote the chemical reactions that cleanse the exhaust. Palladium costs about $50 a gram—more than gold—and each catalytic converter contains about 5 grams of it. Metals like palladium are catalysts—a special class of materials that speed up chemical reactions but don't chemically change themselves. In theory, catalysts can be used over and over, indefinitely. In practice, however, the performance of catalysts degrades over time. To compensate, we are forced to use more of these expensive metals up front, adding to the cost. Our goal is to better understand the causes of this degradation and how to counteract it.

Why do catalysts go bad?

Ideally, catalysts should be designed to have the greatest surface area possible to promote the greatest number of chemical reactions. So, manufacturers typically spread many small particles over the surface of a new catalytic converter. From past research we know that, over time, the metal atoms begin to move, forming larger and larger particles that offer less surface area, and thus become less effective. We call this clumping process "sintering." To counteract sintering, manufacturers use excessive amounts of metal so that the converter will meet emissions standards for the 10- or 15-year lifespan of a car. Our team has discovered that sintering isn't the only cause of deactivation. In fact, this new deactivation mechanism turns out to be quite the opposite of sintering. Under some circumstances, instead of particles getting larger, they decompose into smaller particles and eventually become single atoms that are essentially inactive. This is a new understanding we believe no one has presented before, and it prompted us to look for an entirely new way to maximize the lifespan and performance of the metals in catalytic converters.

What can we do to make catalysts last longer?

Our research suggests that if we carefully control both the size and the spacing of metal particles, palladium particles will neither sinter into large

clumps nor decompose into single atoms.
Previously, many people in the catalysis community thought that if you want to make particles stable, you had to keep them as far apart as possible to prevent migration of the particles. We confounded this notion by bringing together a collaborative team that studied degradation in a new way. Aaron Johnston-Peck from the National Institute of Standards and Technology used advanced microscopy to help visualize the presence of the single atoms. Simon Bare from the SLAC National Accelerator Laboratory used X-ray techniques to prove that catalytic materials start as particles and end up as single atoms. To put these experimental results in a theoretical framework, we worked with Frank Abild-Pedersen from the SUNCAT Center for Interface Science and Catalysis and SLAC, and Philipp Plessow from the Karlsruhe Institute of Technology in Germany. They had the computational resources to help us simulate the deactivation mechanism at the atomic scale. In the end, we've provided a scientific basis that could make it possible to maintain pollution reduction while using less precious metal and lowering the costs of catalytic converters. If automotive engineers ultimately confirm and implement these findings, it would be a huge win for consumers in the long run.

More information: Emmett D. Goodman et al. Catalyst deactivation via decomposition into single atoms and the role of metal loading, *Nature Catalysis* (2019). DOI: 10.1038/s41929-019-0328-1

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