Exploring the potential of single-atom catalysts

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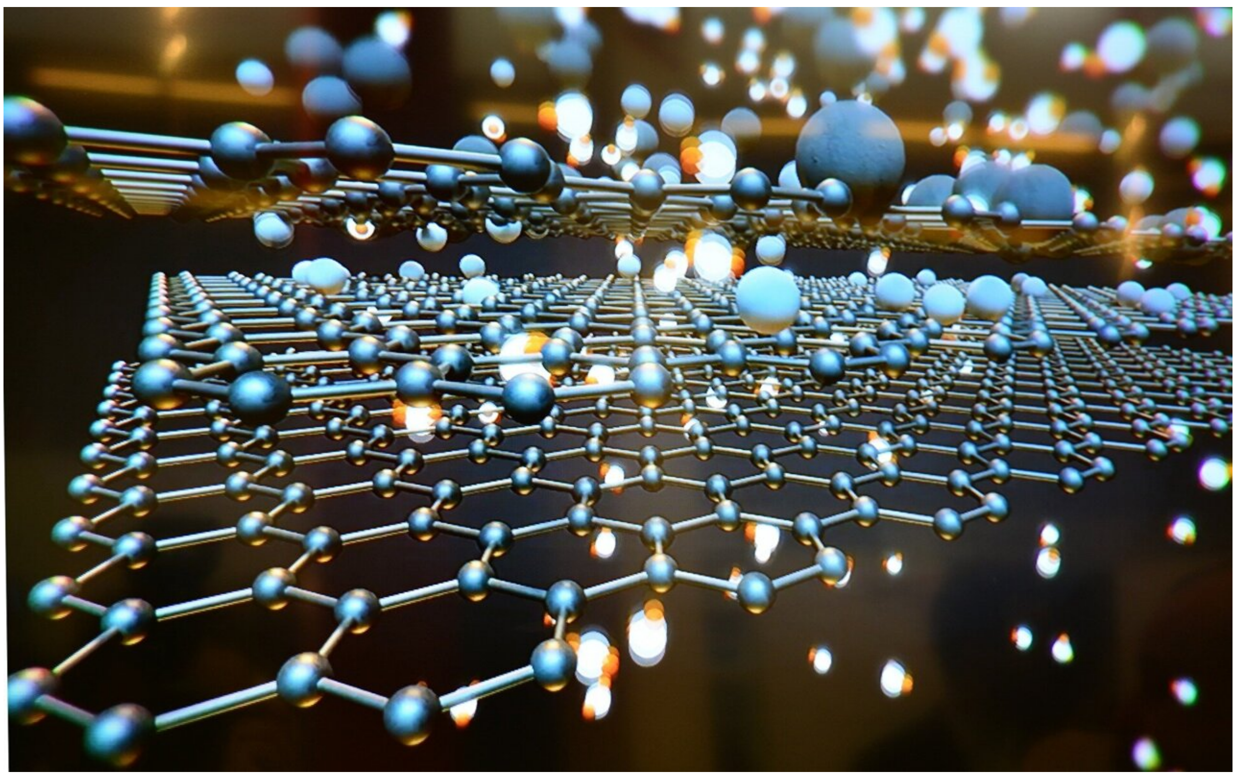

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There is a high level of interest, even excitement, among chemists and materials scientists about the potential of single-atom catalysts (SACs), but their development relies on very specialized tools available only at synchrotrons like the Canadian Light Source (CLS) at the University of

Saskatchewan (USask).

"This is a really exciting research area," said Dr. Peng Zhang, professor of chemistry and biomedical engineering at Dalhousie University and a long-time CLS user.

Catalysts are nanoparticles coated with materials—often expensive metals like platinum, palladium, and gold—that speed up chemical reactions. A significant drawback for conventional catalysts is that only a small percentage of the catalytic material is used in the chemical reaction, making them inefficient and wasteful, explained Zhang.

With the growing demand for clean and sustainable energy, using SACs in energy systems can help the environment and save money. SACs have benefits like making reactions more efficient, using less rare metals, and improving the performance of devices like fuel cells and batteries. They can also help store renewable energy from sources like the sun and wind, making it more reliable.

In the case of automotive catalytic converters, which are designed to convert exhaust emissions into less toxic pollutants, Zhang said less than half of the platinum atoms in the catalyst are available for the necessary chemical reaction.

The goal of SAC research is to control the surface atomic structure of catalysts with individual atoms of the catalytic material in a matrix of less expensive material, ensuring all of the material is available for the reaction. "When you design the catalyst to have a single-atom structure, you can significantly improve their activity and performance in the catalytic application," said Zhang.

The challenges of working at the level of a single atom are significant, he admitted, but that is where the CLS comes in.

"If you think about single-atom catalysts, they're so small that you need a special research tool to uncover their structure" to understand how the atoms are arranged and what atoms are present. "Even with the most powerful electron microscope, you can probably see an individual atom, but if you're using synchrotron technology, you can get a resolution 100 times smaller."

Zhang started using synchrotron facilities and techniques more than 20 years ago in his materials research as a Ph.D. student at the University of Western Ontario. When the CLS opened in 2004, "I was so excited to know that we have our first Canadian synchrotron," he said. Since then, and like his own Ph.D. supervisor, he has sent his students to the CLS and its partner synchrotron—the Advanced Photon Source (Argonne National Laboratory, near Chicago) to conduct SAC experiments on-site.

From a basic research perspective, Zhang said there remain two big hurdles in the development of single-atom catalysts.

"First, we really want to understand better why some single-atom catalysts are so good, so active, but sometimes they might not be stable after a few hours, so we have to design single-atom catalysts to be active over a long period (of time). There is a lot of work to do with these catalysts to make them more powerful and more usable."

The other challenge is ramping up SAC use to a commercial scale.

"We want to collaborate with people in the chemical industry to find real-world applications," Zhang said. "In the lab, you have very small-scale catalysis, but in the chemical industry, it is a thousand times bigger." The ability to scale up a single-atom catalytic reaction opens the door to "all kinds of chemical industry applications."

While the future potential is exciting, Zhang said fundamental SAC research would be impossible without "access to world-class facilities like the CLS and APS."

The research is published in the journal *Accounts of Chemical Research*.

More information: Ziyi Chen et al, Structural Analysis of Single-Atom Catalysts by X-ray Absorption Spectroscopy, *Accounts of Chemical Research* (2024). DOI: 10.1021/acs.accounts.3c00693

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