

# Researchers study the surfaces of ceria nanoparticles

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At Karlsruhe Institute of Technology (KIT), scientists have studied ceria nanoparticles with the help of probe molecules and a complex ultrahigh vacuum-infrared measurement system and obtained new insights into their surface structure and chemical activity. Their work is reported in three articles published in the journal *Angewandte Chemie*.

Cerium oxides, compounds of [oxygen](#) and the rare-earth metal cerium, are among the most important oxides for technical applications. Ceria is mainly used in heterogeneous catalysis, examples being exhaust gas catalytic converters of passenger cars, photocatalysis in solar cells, water splitting, or the decomposition of pollutants. Ceria, as used in catalytic converters, is in the form of a powder. It consists of nanoscaled particles of highly complex structure. Special arrangement of the metal and oxygen atoms on the surface determines the physical and chemical properties of ceria. So far, however, it has been impossible to precisely analyze the rearrangement and reconstruction processes taking place at the surface of the [nanoparticles](#).

At KIT, scientists of the Institute of Functional Interfaces (IFG) under the direction of Professor Christof Wöll established a new method to study chemical properties of oxide surfaces in recent years. They used small molecules, such as carbon monoxide (CO), molecular oxygen (O<sub>2</sub>), or nitrous oxide (N<sub>2</sub>O), as probe molecules. These molecules attach to the surface of the oxide nanoparticles. Then, the researchers determine vibration frequencies of the probe molecules. "This approach has led to major progress in the understanding of surface properties of

ceria nanoparticles," Christof Wöll says.

Together with scientists of the Institute of Catalysis Research and Technology (IKFT) of KIT, Humboldt-Universität zu Berlin, the University of Udine/Italy, and the Polytechnical University of Catalonia in Barcelona/Spain, the IFG researchers studied various aspects of the [surface structure](#) and chemical activity of ceria nanoparticles.

The main reason of the progress achieved is that the researchers succeeded in verifying the vibration frequencies measured for the powders by measurements using exactly defined model substances. They applied a unique ultrahigh vacuum-infrared system. Additionally, they used quantum mechanics calculations to allocate the previously unknown vibration bands of the oxide particles. In this way, they gained entirely new insights into the surface chemistry of ceria nanoparticles.

The scientists proved that the [surface](#) of a bar-shaped ceria nanoparticle has a number of defects, such as sawtooth-shaped nanofacets, [oxygen vacancies](#), corners, and edges. These irregularities probably lead to the high catalytic activity of such nanoparticles. In addition, the researchers found that photoreactivity of ceria can be enhanced considerably by the generation of oxygen vacancies, i.e. unoccupied oxygen sites. Another study yielded basic information on the position of oxygen vacancies on various ceria surfaces and their relevance to oxygen activation. "Based on our findings, we can now systematically further develop and optimize nanoscaled ceria-based [catalytic converters](#) and photocatalysts," Professor Wöll says.

**More information:** Chengwu Yang et al. Surface Faceting and Reconstruction of Ceria Nanoparticles, *Angewandte Chemie International Edition* (2016). [DOI: 10.1002/anie.201609179](https://doi.org/10.1002/anie.201609179)

Chengwu Yang et al. O<sub>2</sub> Activation on Ceria Catalysts - The Importance

of Substrate Crystallographic Orientation, *Angewandte Chemie International Edition* (2017). [DOI: 10.1002/anie.201709199](https://doi.org/10.1002/anie.201709199)

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