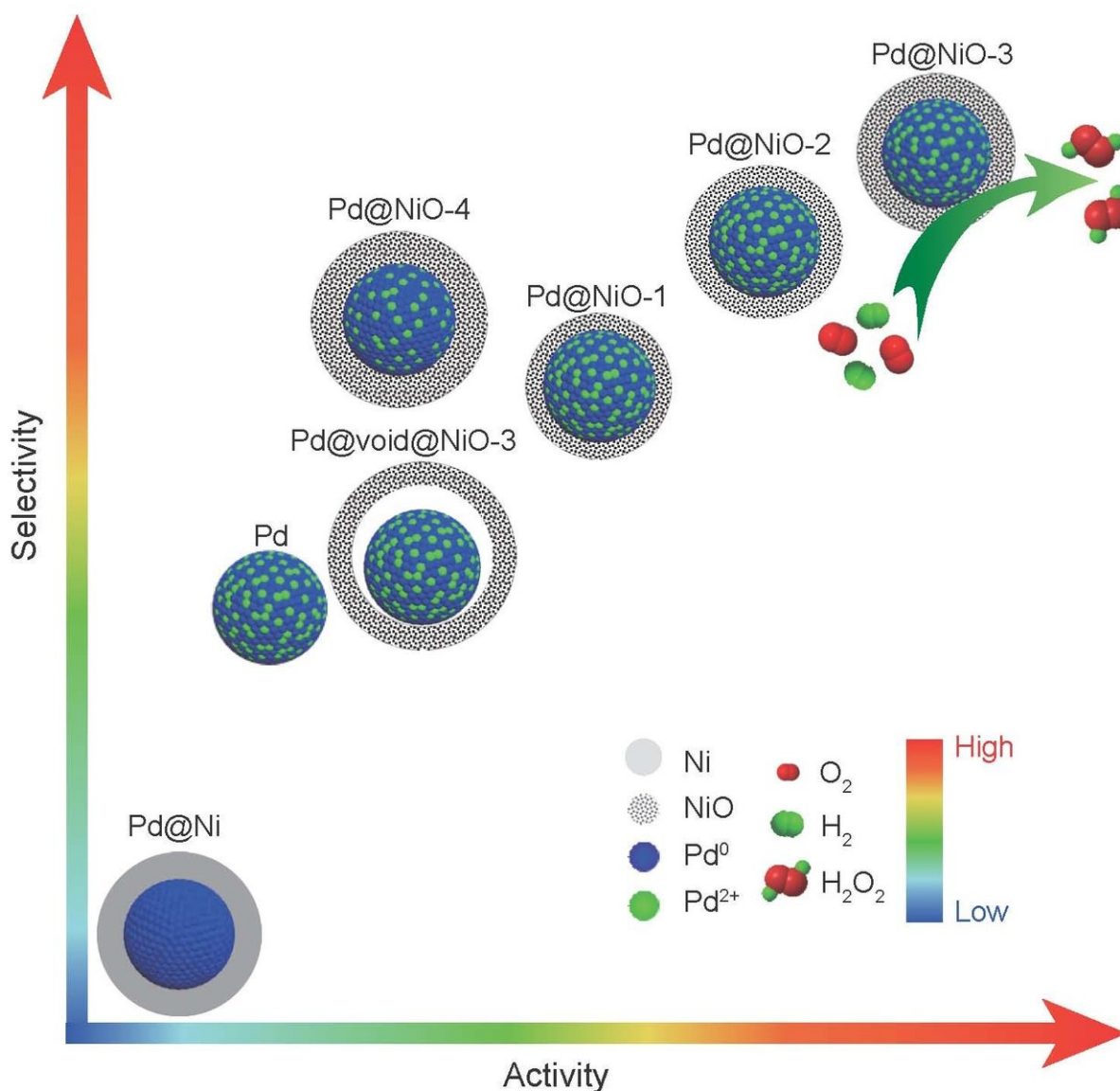


Interfacial engineering core@shell nanoparticles for active and selective direct H₂O₂ generation

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Schematic illustration showing the activity and selectivity toward H₂O₂ synthesis of 5 wt% Pd@Ni-3/TiO₂, 5 wt% Pd@NiO-x/TiO₂ (x = 1, 2, 3, 4), 5 wt% Pd@void@Ni-3/TiO₂ and 5 wt% Pd/TiO₂. Credit: Science China Press

A class of supported Pd@NiO-x core@shell catalysts have been constructed for direct H₂O₂ generation. The optimized Pd@NiO-3/TiO₂ exhibited high activity, superior selectivity, low degradation activity and excellent stability. The unique, cavity-contained interface structure can suppress the overbinding between Pd-core and (O-O)*, which is effective to prevent H₂O formation and guarantees high selectivity of H₂O₂. The present work highlights the importance of interface engineering of Pd-based catalysts for direct H₂O₂ synthesis.

Hydrogen peroxide (H₂O₂) is a versatile chemical, widely applied in modern industry. To date, H₂O₂ is industrially manufactured by an indirect process that involves the sequential hydrogenation and oxidation of alkyl anthraquinone, an energy-intensive, multi-step process with high cost. By contrast, the direct synthesis of H₂O₂ from H₂ and O₂ is expected to be the most efficient way to produce H₂O₂ due to the remarkable advantages of atom economy, low energy consumption and H₂O as its only byproduct.

Currently, the direct synthetic route is mainly achieved by the supported Pd-based catalysts. The major problem associated with that is related to the low selectivity of H₂O₂. Despite great efforts devoted to constructing Pd-based catalysts, understanding high-performance Pd-based catalysts for direct H₂O₂ generation from either deep characterization or theoretical investigation are still extremely limited.

In a new overview published in the Beijing-based *National Science*

Review, scientists at the Soochow University present the latest advances in direct H_2O_2 generation. Co-authors Yonggang Feng, Qi Shao, Bolong Huang, Junbo Zhang, and Xiaoqing Huang developed a class of Pd@NiO-x nanoparticles with a unique core@shell interface structure, which achieves high activity, selectivity and stability for the direct H_2O_2 synthesis.

These scientists interpreted the mechanism from both electronic and energetic views. "Traditional Pd-based catalysts are very active for the side reactions, such as the decomposition and hydrogenation of H_2O_2 as well as the formation of H_2O ," they state in an article titled "Surface engineering in the interface of core/shell nanoparticles promotes [hydrogen peroxide](#) generation."

"It is considered that the intrinsic surface property of Pd-based catalysts is essential for the selectivity and activity of the direct H_2O_2 synthesis," they add. "This arises because the barrier for O-O bond scission is sensitive to Pd surface structure, the key parameter governing H_2O_2 synthesis and decomposition activity."

The creation of porous NiO shell is beneficial for exposing Pd active sites and thus enhancing the productivity of H_2O_2 . "By tuning the composition of Pd@NiO-x NPs and the reaction condition, the efficiency of H_2O_2 synthesis could be well optimized with 5 wt% Pd@NiO-3/TiO₂ exhibiting the highest productivity (89 mol/(kgcath)) and selectivity (91%) to H_2O_2 as well as excellent stability," they state.

"The first principles simulations further revealed the mechanism from both electronic and energetic views," the scientists wrote. "The superiority in selectivity is achieved by a spontaneous bond scission of H-H and charge transfer from O₂₀ to O₂₂- within the cavity of NiO interfacing with Pd surface. (...) The high selectivity and activity make it one of the best catalysts for the direct H_2O_2 synthesis reported to date,"

they add. "The present work reported here highlights the importance of surface and interface engineering of Pd-based catalysts for the direct H₂O₂ synthesis with largely enhanced activity and selectivity."

More information: Yonggang Feng et al, Surface engineering at the interface of core/shell nanoparticles promotes hydrogen peroxide generation, *National Science Review* (2018). [DOI: 10.1093/nsr/nwy065](https://doi.org/10.1093/nsr/nwy065)

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