Efficient and durable water splitting in acidic media

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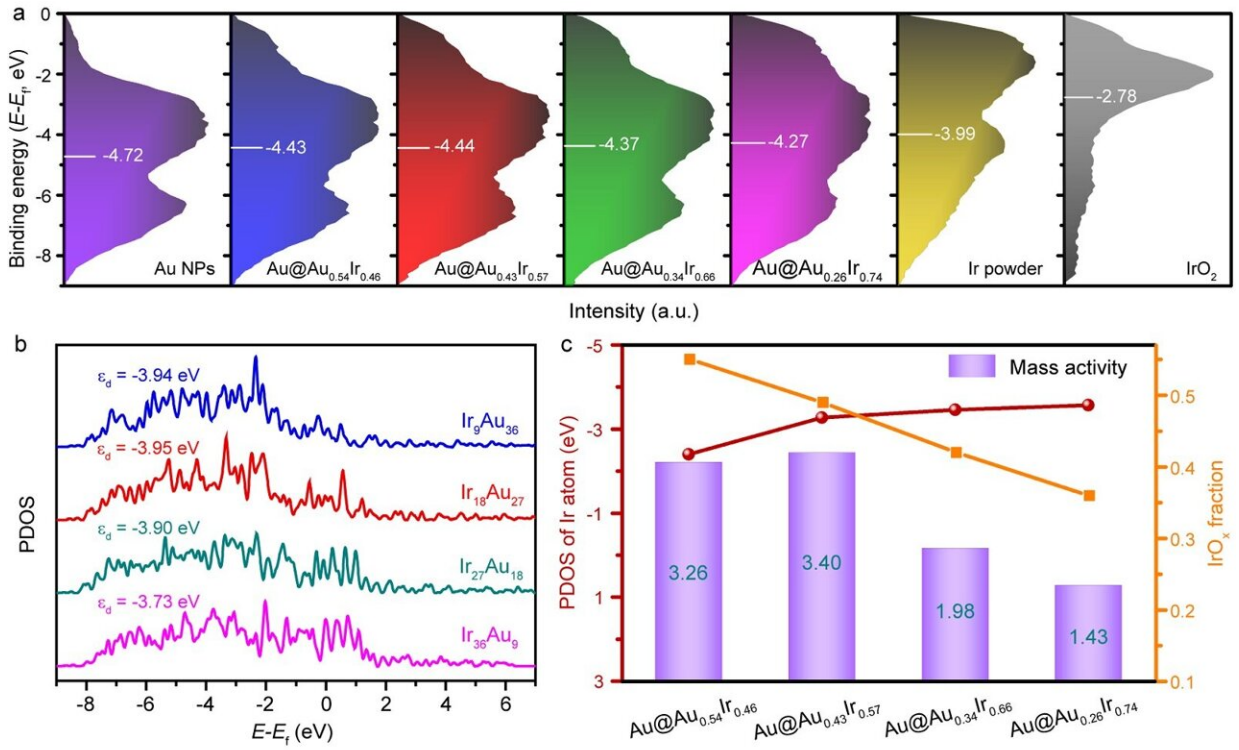


(a) Valence band photoemission spectra of $Au@Au_xIr_{1-x}$ and standard samples. The white bar represents the *d*-band center. (b) DFT calculated PDOS of *d* -bands and *d*-band centers for Au-Ir systems. (c) Structure-activity relationships. Credit: Science China Press

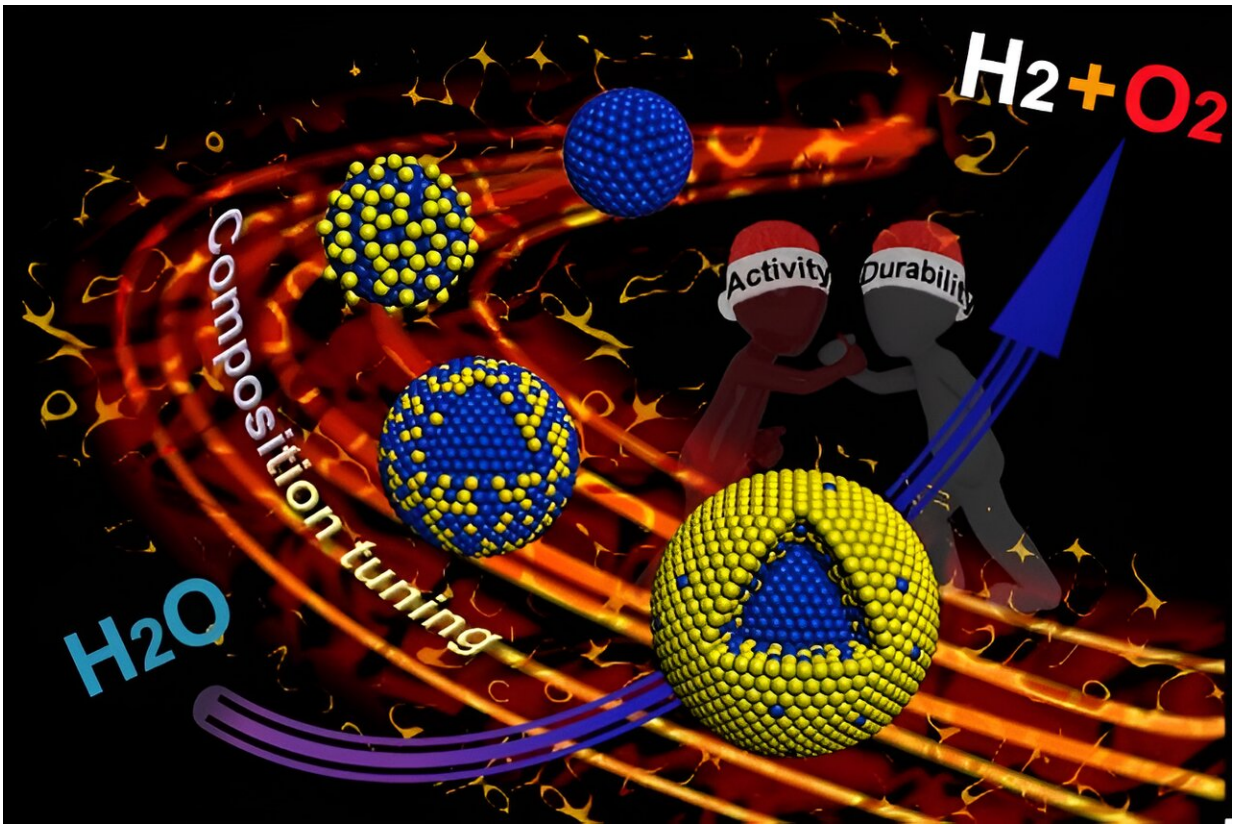
Recent research published in *National Science Review* by a team led by Dr. Rong Cao and Dr. Minna Cao from the Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, and Dr. Dongshuang Wu from Nanyang Technological University, Singapore, has demonstrated the successful design and synthesis of a series of sub-10 nm core-shell nanocatalysts consisting of an Au core and an Au_xIr_{1-x} alloy shell.

The first author Dr. Huimin Wang successfully synthesized and systematically tested the electrocatalytic water-splitting performance of this series of materials.

Dr. Huimin Wang found that the active site IrO_x can be precisely designed by modulating the Au/Ir component on the surface of the $Au@Au_xIr_{1-x}$ core-shell structure. IrO_x species on the $Au@Au_xIr_{1-x}$ surface is generally considered the active species for OER.

However, an excessive amount of IrO_x shifts the d-band center of the catalyst close to the Fermi level, causing a too-strong binding affinity of intermediates that needs a quite high overpotential for the OER. Synchrotron X-ray-based spectroscopies, electron microscopy, and density functional theory calculations combined with electrochemical tests revealed that an optimal ratio of IrO_x combined with a suitable d-band center yields the best OER activity.

Among them, the intrinsic activity and durability of $Au@Au_{0.43}Ir_{0.57}$ are substantially improved. With a load of only 0.02 mg_{Ir}/cm^2, it is stable for at least 320 h at a high current density of 100 mA/cm^2.



Surface active and durable IrO_x is precisely controlled by tuning Au/Ir compositions, which can realize a balance for activity and stability for water splitting. Credit: Huimin Wang.

More information: Huimin Wang et al, Sub-10-nm-sized Au@AuxIr1−x metal-core/alloy-shell nanoparticles as highly durable catalysts for acidic water splitting, *National Science Review* (2024). DOI: 10.1093/nsr/nwae056

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