Researchers develop catalyst for stable reduction of carbon dioxide

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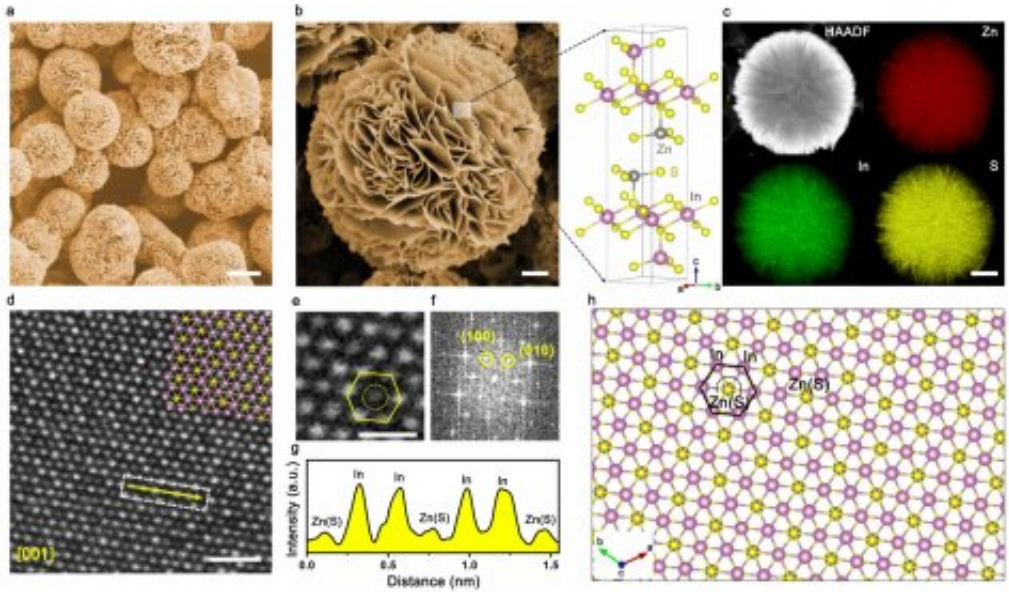

Structure characterization of catalyst. Credit: Chi Liping et al.

Electrocatalytic carbon dioxide reduction (CO_2RR) is an effective means of CO_2 resource utilization. The current developed catalysts can effectively catalyze CO_2RR to prepare a variety of carbon-based fuels such as formic (HCOOH) which is most likely to be commercialized in the future.

However, the current catalyst present particle agglomerate, active-phase change and element dissolution during the high-speed electrolysis, resulting in the rapid drop of HCOOH selectivity. It is necessary to

develop catalysts with both activity and stability to realize the industrial preparation of electrocatalytic CO_2 to HCOOH.

A research team led by Prof. GAO Minrui from University of Science and Technology of China (USTC) of the Chinese Academy of Sciences stabilized the catalyst structure by strengthening the covalent property of materials. With the obtained indium sulfide catalyst, the selectivity of formic acid product can remain about 97%. This work was published in *Nature Communications*.

The researchers improved the covalence of indium sulfur bond and effectively inhibited the loss of active component, sulfur, in the catalyst by introducing zinc (Zn) into indium sulfide. Utilizing the same synthesis strategy, they prepared In_2S_3 and $ZnIn_2S_4$ catalysts to explore its efficiency.

Electrochemical performance test showed that the structure of $ZnIn_2S_4$, modulated by Zn, presented great $HCOO^-$ Faraday efficiency and partial current density in neutral electrolytic environment. In particular, the incorporation of Zn enabled $ZnIn_2S_4$ to have excellent catalytic stability. In the uninterrupted continuous electrolysis process, the catalyst could stably catalyze the formation of $HCOO^-$ at industrial current density over 60 hours, and maintain the Faraday efficiency at about 97%.

Furthermore, the researchers conducted rigorous structural stability tests on the catalyst. Through X-ray diffraction and scanning electron microscopy, they found that the phase and morphology of $ZnIn_2S_4$ catalyst were well maintained even when the current density was relatively higher. Whereas, In_2S_3 was completely transformed into a metallic In, and S was completely lost at relatively low current density. In this condition, the loss of S led to the complete structure collapse.

They also used X-ray photoelectron spectroscopy and STEM-EDX

elemental analysis to confirm the serious loss of S of In_2S_3 during electrolysis. On the contrary, the content and chemical state of each element (Zn, ln and Si) in $ZnIn_2S_4$ structure hardly changed. With the help of computer simulation, they found that in $ZnIn_2S_4$, the bond fracture between in ln(Zn) and S was unfavorable in dynamics and the dissolution of S element was blocked. This simulation result explained the internal mechanism of high current electrolysis stability.

This work improved the internal stability of the catalyst by introducing foreign elements to enhance the covalency of the material, which provides a new idea for the design and creation of CO_2RR catalyst for long-time industrial preparation.

More information: Li-Ping Chi et al, Stabilizing indium sulfide for CO2 electroreduction to formate at high rate by zinc incorporation, *Nature Communications* (2021). DOI: 10.1038/s41467-021-26124-y

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