

# Researchers realize paired electrosynthesis of dimethyl carbonate with single-atom catalyst

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Illustration of the research. Credit: Prof. Zhu's group

Typically in a traditional electrochemical cell with a membrane separator, the products of cathodic  $\text{CO}_2$  reduction reaction ( $\text{CO}_2\text{RR}$ ) are usually in reduced forms. The anodic  $\text{O}_2$  evolution does not play a role in further expanding the product scope.

Dimethyl carbonate (DMC,  $\text{CH}_3\text{OCOOCH}_3$ ) is an environmental-benign chemical feedstock. The convergent paired [electrosynthesis](#) of DMC represents an important revolution for the DMC production.

In a study published in *Energy & Environmental Science*, a research group led by Prof. Zhu Qilong's group from Fujian Institute of Research on the Structure of Matter of the Chinese Academy of Sciences reported an Ni single-atom catalyst (Ni SAC) for  $\text{CO}_2$ -to-CO conversion and the convergent paired electrosynthesis of DMC.

The researchers found that the convergent paired electrosynthesis couples the anodic halide ion oxidation reaction and the cathodic  $\text{CO}_2$ RR to generate the key intermediates for the DMC synthesis. During this conversion, the efficient cathodic  $\text{CO}_2$ -to-CO conversion plays a dominant role, inspiring great effort to control the micro-nanostructure of electrocatalysts.

They also revealed that the dual-channel superstructured Ni SAC with a unique site coordination configuration bonded via one axial oxygen atom and four planar nitrogen atoms is controllably constructed and is capable of providing a preeminent performance for  $\text{CO}_2$ -to-CO conversion, achieving the exclusively high Faradaic efficiency (FE) and partial current densities with excellent stability.

By virtue of the atomic to nanoscopic to microscopic manipulation of the penta-coordinated Ni SAC for CO production, the convergent paired electrosynthesis of DMC from  $\text{CO}_2$  was pioneeringly performed, realizing the high FE of DMC.

The mechanism study unveiled that such axial oxygen coordination configuration is helpful to decrease the [energy](#) barriers for the generation of key  $^*\text{COOH}$  intermediate and the dissociation of  $\text{H}_2\text{O}$  and  $\text{CH}_3\text{OH}$ , accelerating the convergent paired electrosynthesis.

This study suggests that the proof of concept in the innovative convergent paired electrosynthesis could open up a new horizon in the fields of CO<sub>2</sub> utilization.

**More information:** Xiaofang Li et al, Convergent paired electrosynthesis of dimethyl carbonate from carbon dioxide enabled by designing the superstructure of axial oxygen coordinated nickel single-atom catalysts, *Energy & Environmental Science* (2022). [DOI: 10.1039/D2EE03022E](https://doi.org/10.1039/D2EE03022E)

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