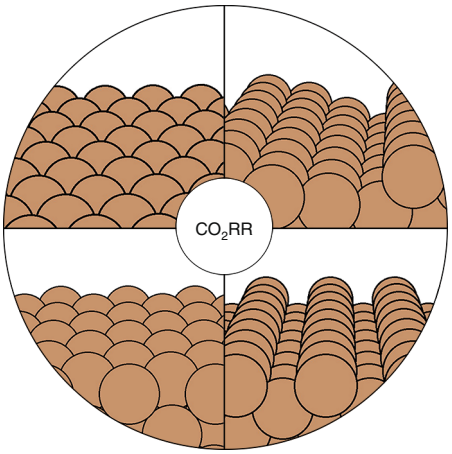
CARBON DIOXIDE ELECTROREDUCTION

The many faces of copper

ACS Catal. **9**, 7894–7899 (2019).



The electrochemical reduction of carbon dioxide has received a great deal of attention for decades, on one hand because it would enable the production of fuels and chemicals by using renewable electricity and on the other, because it could help diminish global warming. While some metals are able to achieve almost full Faradaic efficiency to C_1 products — for example, Ag or Au to carbon monoxide, or Sn or In to formic acid, Cu is the only metal that promotes C–C coupling and can exhibit Faradaic efficiencies for multicarbon products as high as 80–90%. This is due to the ability of copper to bind carbon monoxide without having an underpotential deposition of hydrogen. Nevertheless, multicarbon products include a whole range of species and the selectivity trends among the many copper-based catalysts remain still largely unexplored.

Now, Alexander Bagger and Jan Rossmeisl at University of Copenhagen, in collaboration with researchers in Germany and Mexico, make use of the early works by Yoshio Hori and colleagues on copper single-crystals to elucidate trends among the products and structural features of the catalysts, without explicitly considering the complex reaction network of carbon dioxide reduction. The original dataset from Hori's work contains 20 catalyst surfaces and up to 10 products of the targeted reaction, plus hydrogen from the competing hydrogen evolution reaction. To this end, the researchers perform correlation and principal component analyses on datasets comprising the products' Faradaic efficiency, facets' coordination number and binding energy of certain species.

While the common C_{2+} product formations tend to correlate with each other, some exceptions are observed, such as acetic acid and acetaldehyde, which correlate with each other and also with CO. Likewise, a coordination number of eight correlates with C_{2+} products besides the aforementioned two, which correlate with a coordination number of seven, similar to the oxygen-containing C_1 species. The principal component analyses show that for each dataset, two principal components capture 70–80% of the variance. (100) basal planes promote C_{2+} Faradaic efficiency, which is further enhanced by the presence of defects such as steps. In particular, the (100)x(110) step promotes ethanol formation.

Marçal Capdevila-Cortada

Published online: 13 September 2019
https://doi.org/10.1038/s41929-019-0356-x