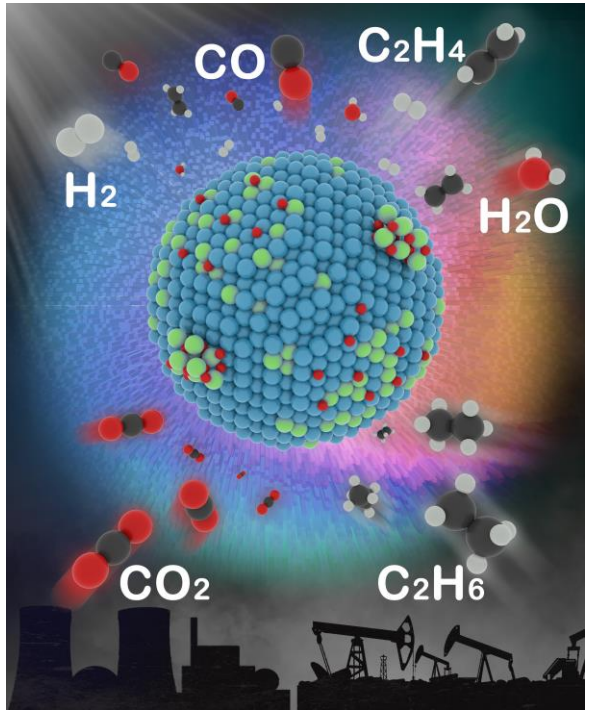
Steering the Conversion of CO_2 and Ethane



The illustration shows the catalyst and the various products it can help create.

Scientific Achievement

Scientists identified key catalytic features to drive the transformation of carbon dioxide (CO_2) with help from ethane into higher-value chemicals.

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Significance and Impact

In this study, the researchers solved the challenge of discovering the right catalytic pathway to convert CO_2 using ethane to gas for generating electricity, liquid fuels, or ethylene.

Research Details

- Discovered two descriptors to control the selectivity of the C_2H_6−CO_2 reaction to favor one catalytic reaction product.
- Performed X-ray studies at the ISS & QAS beamlines at NSLS-II & 17-BM-B at APS.
- Used materials characterization & computational tools at the CFN as well as computational resources at NERSC.

Z. Xie, X. Wang, X. Chen, P. Liu, J. G. Chen, *JACS*, **144** (9), 4186-4195 (2022).

Work was in part performed at Brookhaven, Argonne, and Lawrence Berkeley National Laboratories