## Dual Single Atom Catalysts for Highly Selective CO<sub>2</sub>-to-C<sub>2</sub> Conversion

Soressa Abera Chala,<sup>1</sup> and <u>Bing Joe Hwang</u>\*<sup>1,2,3</sup>

<sup>1</sup> Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan; <sup>2</sup>Sustainable Electrochemical Energy Development (SEED) Cener, National Taiwan University of Science and Technology, Taipei, Taiwan; <sup>3</sup>National Synchrotron Radiation Center, Hsin-Chu, Taiwan Email: bjh@mail.ntust.edu.tw

The electrochemical CO<sub>2</sub>-to-C<sub>2</sub> conversion bargains a promising approach to lowering CO<sub>2</sub> emission while yielding valuable chemical products. Here, we report the NiCu-SACs/N-C catalysts<sup>[1]</sup> with cooperative dual heteroactive sites that achieve by far the highest catalytic activity for yielding ethanol with the unprecedented Faradaic efficiency of 92.2% at the potential of -0.6 V versus RHE. The catalyst exhibits the lowest onset potential of -0.4 V versus RHE to catalyze CO<sub>2</sub>-to-C<sub>2</sub> conversion. In-operando X-ray absorption spectroscopy provides an interesting observation of restructuring behavior of dynamically generated Cu clusters from atomically distributed Cu single-atoms and reversible structural changes or oxidation states of Cu sites while Ni sites remain unchanged during the catalytic reactions. Our experimental analysis and DFT computation suggest that CO produced on Cu-N4/Ni-N3 cooperative single atom sites undergoes C-C coupling, which is further reduced into ethanol. This strategy provides a new route to design selective and efficient catalysts for CO<sub>2</sub>-to-C<sub>2</sub> conversion.



## References

1. Chala S. A. et al., Applied Catalysis B: Environment and Energy, 2024, 358, 124420.