Advancements in Surface and Structural Engineering on Electrocatalysts for Enhanced CO2 Reduction Reaction

Kuan-Wen Wang
Full Professor, Institute of Materials Science and Engineering, National Central University, Taoyuan, Taiwan

Wan-Chun Huang
Institute of Materials Science and Engineering, National Central University, Taoyuan, Taiwan

Wei-En Yang
Institute of Materials Science and Engineering, National Central University, Taoyuan, Taiwan

Abstract:

The electrochemical reduction of carbon dioxide (CO2RR) presents a promising pathway for producing industrial chemicals using renewable electricity. Accelerating the deployment of CO2RR technologies requires the development of highly selective, durable, and cost-effective catalysts. This study demonstrates that Cu-based catalysts modified with AuCu shell, or In2O3 interfaces exhibit significantly enhanced selectivity and stability for CO2-to-CO conversion compared to pure Cu or reference catalysts. Au2-Cu8 alloyed core-shell catalyst (only 17% Au content) achieves a CO faradaic efficiency (FECO) of 94% at -0.8 V while Cu-In2O3 catalyst, in which a low amount of In2O3 decorated on Cu surface, achieves a FECO of 95% at -0.7 V. Theoretical calculations corroborate these findings, revealing that the CuAu and In2O3 components play crucial roles in lowering the energy barrier for the formation of key reaction intermediates. Collectively, our results highlight the potential of these engineered Cu-based catalysts for the efficient electrochemical conversion of CO2 to CO, paving the way for sustainable industrial chemical production powered by renewable energy.

Keywords:

CO2 reduction reaction, copper, indium oxide, gold, density functional theory.