

Unraveling the reactive site mechanism of the electrochemical CO₂ reduction on CoPc

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High efficient carbon dioxide to chemical fuel is a promising route to utilize excessive released CO₂ and ultimately leading to a carbon neutral energy cycle. Electrochemical CO₂ reduction is of particular interest as it demands less harsh reaction condition and is capable of coupling with renewable energy source such as wind and solar energy. Cobalt phthalocyanine (CoPc) as a typical transitional metal complex catalyst for electrochemical CO₂ reduction is able to convert CO₂ to CO with high selectivity and activity. These features make CoPc an ideal model catalyst for studying the reaction mechanism of CO₂RR. Because of the potentials at which multiple reduction product is produced lies within a relative narrow window, it is unlikely to control the products through thermodynamic approaches. Therefore, the good CO selectivity property of CoPc is presumed to originate from kinetics reasons. Herein, XPS and soft X-ray absorption spectroscopy were employed to elucidate the catalytic active site evolution during the reaction process. Spectroscopic calculations were also conducted to confirm these discoveries.