Highly Selective CH_4 production by Photocatalytic CO_2 Reduction using a Zn-based Polyoxometalate

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Photocatalytic CO_2 reduction reaction (CO2RR) to CH_4 is a promising method to solve energy and climate change problems. However, it is difficult to increase both the efficiency and selectivity for CO2RR due to high energy consumption, various reaction pathways, and a competitive reaction. Here, we report the synthesis of Zn-based polyoxometalate (ZnPOM) and its application in highly selective photochemical CO2RR for CH_4 production. Whereas Zn-based catalysts are conventionally known to produce CO through CO2RR, ZnPOM selectively produces CH_4 in the presence of an Ir-based photosensitizer (TIr3). We propose the basis for selectively producing CH_4 through photocatalytic CO2RR when ZnPOM was used as a CO2RR catalyst through photophysical and computational analyses: (1) fast charge transfer from TIr3 to ZnPOM through the strong molecular interaction between them; (2) effective electron transfer from ZnPOM to *CO intermediates due to significant hybridization of their molecular orbitals; (3) appropriate strength of *CO binding energy in ZnPOM. This study can provide insights to the design of CO2RR catalysts beyond the conventional limitations that focus on Cu-based materials.