Highly efficient carbon dioxide photoreduction guided by machine learning and first-principles calculation

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BiOBr-Bi-g-C₃N₄ heterojunction with double electron transfer channels was successfully constructed, which can localize the photoexcited carriers at the interlayers rather than randomly distributing, resulting in a 4.7- and 3.1-fold increase compared to Bi-BiOBr and Bi-g-C₃N₄ samples. Credit: Chinese Journal of Catalysis

Photocatalytic reduction of CO₂ to high-value carbon-based fuels holds tremendous potential in addressing the growing energy crisis. However,
the high C=O bond energy of CO$_2$ molecules (750 kJ·mol$^{-1}$) makes it challenging to activate and reduce CO$_2$.

Therefore, the construction of photocatalysts with novel electron transfer pathways is meaningful. Compared with the traditional single electron transfer channel, the development of multi-electron channels based on layered materials has obvious advantages in the improvement of carrier transport. Nevertheless, the rational design of a desirable photocatalytic model for multi-electron channels with optimized parameters is quite challenging.

Recently, a study titled "Constructing dual electron transfer channels to accelerate CO$_2$ photoreduction guided by machine learning and first-principles calculation" was designed and led by Prof. Jizhou Jiang from Wuhan Institute of Technology, China.

This work combines first-principles calculating and machine learning to successfully predict and prepare a novel BiOBr-Bi-g-C$_3$N$_4$ sandwich structure with dual electron transport channels for photocatalytic CO$_2$ reduction. There are three main reasons for the favorable activity by the novel structure:

(1) the introduced g-C$_3$N$_4$ nanosheets demonstrate a similar energy level structure with BiOBr, which benefits for forming an electronic superposition state;

(2) the excited carriers can be efficient separation and transferred owing to the special double electron transfer channels;

(3) since the photo-generated carrier of BiOBr and g-C$_3$N$_4$ have different time decay behavior, a multi-timescale reaction mechanism for CO$_2$ reduction can be constructed to optimize the reaction pathway.
An enhanced photocatalytic performance of CO$_2$ reduction (43 μmol g$^{-1}$ h$^{-1}$) is received by the BiOBr-Bi-g-C$_3$N$_4$ quantum well structure. Five machine learning models were used to explore the linear law of the various influence factors on the efficiency of multi-electron channels. The mechanism of photocatalysis was investigated systematically.

The results were published in *Chinese Journal of Catalysis*.


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