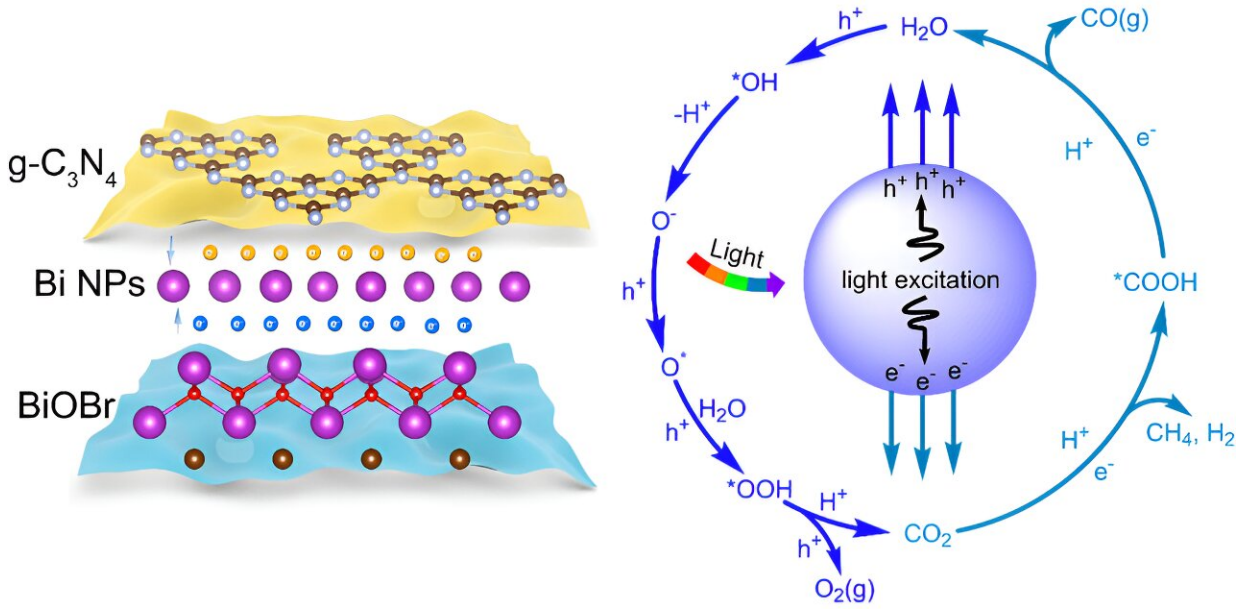
Highly efficient carbon dioxide photoreduction guided by machine learning and first-principles calculation

December 11 2023



BiOBr-Bi-g-C_3N_4 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-C_3N_4 samples. Credit: Chinese Journal of Catalysis

Photocatalytic reduction of CO_2 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 $kJ \cdot mol^{-1}$) 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_3N_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_3N_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_3N_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_3N_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*.

More information: Lijing Wang et al, Constructing dual electron transfer channels to accelerate CO2 photoreduction guided by machine learning and first-principles calculation, *Chinese Journal of Catalysis* (2023). DOI: 10.1016/S1872-2067(23)64546-2