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Photocatalysts for CO2 reduction and computational insights
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Abstract
Global warming is caused by excessive CO2 production, and reducing CO2 emissions is a viable way to counteract this. It has been extensively studied how light-driven processes, particularly photocatalytic systems, can transform solar energy into chemical energy. In the present review exercise, the mechanism of CO2 reduction is described using calculations based on density functional theory (DFT), and comparisons are also made with regard to typical light-driven devices. Additionally, the traits of potential materials—including metal–organic frameworks (MOFs), metal complexes, metal oxide, Z-scheme (metal complexes/semiconductors, two semiconductors, dye-sensitized semiconductors), improved S-scheme and organic photocatalyst etc.—are described in depth to show how these traits affect the CO2 adsorption, activation, and desorption processes. Also summarized are a number of methods for enhancing the selectivity and efficiency of catalytic reactions. Lastly, the challenges and future outlook of light-driven reactions for CO2 reduction are presented.

Author Keywords
CO2 reduction; MOFs; Photocatalysts; S-scheme; Z-schemes

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