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In situ FT-IR investigation on the reaction mechanism of visible light photocatalytic NO oxidation with defective g-C_3N_4

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Abstract: The g-C_3N_4 with different structures was prepared by heat treatment using urea (CN-U) and thiourea (CN-T) as precursors under the same conditions. The microstructure and optical properties of the photocatalyst were analyzed with advanced tools. The results showed that the CN-U has a porous structure, a high specific surface area and a wide band gap in comparison with CN-T. The in situ FT-IR technique was used to monitor the adsorption and reaction process of visible photocatalytic NO oxidation on g-C_3N_4. The corresponding reaction mechanism was proposed based on the results of reaction intermediate observation and EPR radical scavenging. It was revealed that (1) the presence of defective sites favored the adsorption of gas molecules and electronically compensated it leading to promoted formation of the final products; (2) the high separation efficiency of photogenerated electron-hole pairs enhanced the production of radicals during the photocatalytic reaction; (3) the hydroxyl radicals (▪OH) are not selective for the decomposition of pollutants, which are favorable to the complete oxidation of the reaction intermediates. The above three aspects are the main reasons for the CN-U possessing the efficient visible light photocatalytic activity. The present work could provide new insights and methods for understanding the mechanism of photocatalysis.

Keywords: g-C_3N_4; visible light photocatalysis; defects; in situ FT-IR; reaction mechanism