

A Creative Approach to Designing and Synthesizing an Effective Plasmonic Photocatalyst Based on g-C₃N₄

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Plasmonic photocatalysts attract interest because they can efficiently absorb and convert solar energy through the local surface plasmon resonance (LSPR) effect. Numerous silver-based plasmonic photocatalysts have been investigated. However, the silver content was often fairly high, the correlation between the silver content and the plasmon effect is rarely discussed, and the LSPR effect on the photoabsorption process at the molecular level has not been addressed. Our project focuses on enhancing the activity of graphitic carbon nitride (g-C₃N₄) in polluted water treatment through the utilization of silver's LSPR effect. Utilizing a unique approach combining machine learning and computational chemistry, we demonstrated the formation of the Ag/AgCl semiconductor and the synergistic effect between Ag/AgCl and g-C₃N₄. For optimal plasmonic effects, silver content should be low and the Ag: AgCl ratio should be approximately 2:1. Three plasmonic Ag@AgCl/g-C₃N₄ photocatalysts with Ag contents of 0.25%, 1.0%, and 1.5% were successfully synthesized according to theoretical suggestions. The Ag@AgCl/g-C₃N₄ ternary exhibits high porosity and reveals superior photoabsorption. They are highly active in Rhodamine B photodegradation with an efficiency of 99.95% within 60 min under visible light radiation, and the products do not consist of toxic aromatic rings. The plasmon effect was shown to be maximal when the silver content is 1%. The heterojunction structure of Ag@AgCl/g-C₃N₄ prevented the recombination of photo-induced electron-hole pairs, thereby improving the photocatalytic performance. The catalysts are highly reusable. Based on theoretical and experimental results, a mechanism for the photoabsorption process with pH influence was proposed.

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