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Organic and Inorganic Chemistry 2018: The g-C3N4 surface-decorated $Bi_2O_2CO_3$ for improved photo catalytic performance: From theoretical calculation to practical antibiotics photo degradation in actual water-Huiping Zhao-Wuhan Institute of Technology

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To overcome the issue of UV-light response character of $Bi_2O_2CO_3$ due to its wide band gap, we primarily attempted to understand the possibility of improving the photocatalytic activity of $Bi_2O_2CO_3$ via g-C_3N_4 surface decoration by the theoretical calculation. Subsequently, g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ was successfully prepared via a facile hydrothermal method. It was found that the g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ samples exhibited enhanced activities for the photo degradation of tetracycline compared with pure $Bi_2O_2CO_3$ upon simulated solar light irradiation. Among them, the 10 wt% g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ sample showed the highest photo catalytic efficiency. First principle calculation and experimental data confirmed that the charge transfer at the interface between g-C_3N_4 and $Bi_2O_2CO_3$ could significantly suppress the recombination of photogenerated electron-holes pairs, thus improving the photocatalytic performance. The proposed mechanism for the enhanced photocatalytic activity was also discussed. Moreover, the photodegradation of antibiotics over g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ was also performed in actual water matrix.

1. Introduction: The harmful effects of antibiotics in ecosystems have been widely studied in recent years. Among them, tetracycline is one of the most common and widely used antibiotics due to its broad antibacterial spectrum and cheap price. Like other antibiotics, tetracycline residue in waste water could produce potential risks for aquatic and terrestrial ecosystems. Consequently, exploring efficient methodology for the antibiotic tetracycline treatment in waste water has been received particular research attention. There are numbers of traditional techniques for wastewater treatment including biological process, adsorption process, membrane processes and chemical oxidation methods. Correspondingly, some advanced oxidation technologies for water purification are mostly concerned in recent years, which majorly involve electrochemical, photochemical, Fenton, and some combinational processes of them in energy devices. Compared with all the other methods, semi-conductor photo catalysis emerges as a most powerful and cost effective alternative for antibiotics removal in waste water owing to the mineralization of organics by highly effective active species generated in the process.

Experimental:

2.1. Chemicals: Bismuth nitrate pentahydrate (Bi(NO3)3•5H2O), tetracycline (TC),tetracycline hydrochloride (TC•HCl), oxytetracycline (OTC), congo red(CR), methyl orange (MO), malachite green (MG) and methylene blue(MB) were purchased from Aladdin. Urea and melamine were purchased from Sinopharm Chemical Reagent Co., Ltd. (Shanghai, China).All the chemicals were of analytical reagent grade and used without further purification.

2.2. Preparation: Graphitic carbon nitride (g-C3N4) was prepared according to the literature. Typically, 10 g melamine were placed into a semi-closed combustion boat, which was heated in a program-controlled muffle furnace to 500 °C at a rate of 5 °C min−1and then kept at that temperature for 2 h. Subsequently, the obtained sample was collected by cooling naturally to room temperature

2.3. Characterization: Powder X-ray diffraction (XRD) was carried on Bruker axs D8Discover (Cu Ka = 1.5406 Å). The scanning rate was 1° min−1in the 2θrange from 10° to 80°. Scanning electron microscopy (SEM) images were taken on Hitachi S4800 scanning electron microscope operating at5 kV. Transmission electron microscopy (TEM) images were recorded on a Philips Tecnai 20 electron microscope at an accelerating voltage of200 kV. More experimental conditions are Photocatalytic activity evaluation, electrochemical measurement and First-principle calculation.

Results and Discussion:

3.1. First principle calculation and band structure analysis In order to understand the possibility of the improved photocatalytic properties of $Bi_2O_2CO_3$ via g-C_3N_4 surface-decoration, the thermodynamic stability and the charge transfer at the interface between g-C_3N_4 and $Bi_2O_2CO_3$ were primarily investigated. The optimal calculation results of different random initial models all end up with g-C_3N_4 lying on $Bi_2O_2CO_3$ (0 0 1) facet. The interface formation energy was calculated according to the following equation: E E F g C N BOC = 3 4/ (001) E E g C N BOC 3 4 (001) where EF is the formation energy, Eg C N BOC 3 4/ (001), Eg C N3 4 and EBOC (001) represent the total energy of the optimized g-C_3N_4 /BOC(0 0 1) model, monolayer g-C_3N_4 and $Bi_2O_2CO_3$ (0 0 1) slab, respectively.

3.2. Characterization of g-C_3N_4 / $Bi_2O_2CO_3$ samples Based on the theoretical calculation, surface-decorated $Bi_2O_2CO_3$ samples with different g-C_3N_4 amount (4.8, 10, and 33.3 wt%) were prepared. XRD patterns of g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ samples. All the diffraction peaks of g-C_3N_4 decorated $Bi_2O_2CO_3$ samples could be well matched to the standard diffraction data of tetragonal $Bi_2O_2CO_3$ (JCPDS card No. 41-1488), indicative of the formation of tetragonal $Bi_2O_2CO_3$

phase. In order to confirm the presence of g-C_3N_4 in the surface-decorated $Bi_2O_2CO_3$ sample, FT-IR spectra of g-C_3N_4, $Bi_2O_2CO_3$, and g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ samples were characterized.

3.3. Photocatalytic activity evaluation

The variations of TC concentrations (Ct/Co) with irradiation time during the photocatalytic process, where Co is the initial TC concentration and Ct is the TC concentration at t time. Direct photolysis of TC could be negligible upon solar light irradiation. It was found that all the g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ samples exhibited higher photocatalytic activity than that of bare $Bi_2O_2CO_3$. The good linear relationship indicates that the process follows the traditional Langmuir-Hinshelwood (L-H) mechanism.

4. Conclusion :

In summary, we clarified the charge transfer process at the interface of g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ photocatalyst through the first principle simulation and band match analysis, which confirmed the possibility of enhancing the photocatalytic activity of $Bi_2O_2CO_3$ through g-C_3N_4 surface-decoration. The g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ samples were prepared via a facile hydrothermal method. Based on the electrochemical measurement and PL spectra, the relatively faster charge transfer rate combined with the deeply suppressed recombination of photo-generated electron-hole pairs greatly facilitate the enhancement of photocatalytic efficiency of the g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ photocatalyst. Moreover, the photocatalytic activity of the g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ sample for TC degradation in actual water matrix was also evaluated. This work not only provides a new route to fabricate g-C_3N_4 surface-decorated $Bi_2O_2CO_3$ photocatalyst, but also develops a strategy to improve the photocatalytic performance for UV light response semiconductor photocatalysts.

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