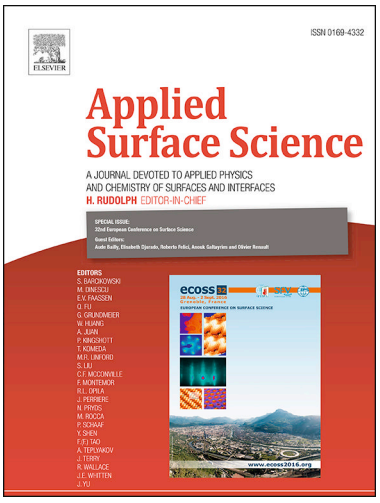

Full Length Article

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Photocatalytic water splitting of (F, Ti) codoped heptazine/triazine based g-C_3N_4 heterostructure: A hybrid DFT study

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ABSTRACT

Graphitic carbon nitride (g-C_3N_4) has been widely investigated as a metal-free photocatalyst for water splitting. However, the rapid recombination of photoexcited carriers and narrow visible-light response region substantially limit its performance. In this work, we have systematically studied the geometrical, electronic, optical, charge transfer and photocatalytic mechanism of (F, Ti) codoped heptazine/triazine based g-C_3N_4 heterostructure using hybrid density functional approach. The interface interaction between heptazine and triazine g-C_3N_4 shows heptazine and triazine g-C_3N_4 form a Van Der Waals heterostructure. The bandgap of (F, Ti) codoped heptazine/triazine based g-C_3N_4 heterostructure is narrow (2.39 eV), which enhances the absorption of visible light and leads to an obvious redshift of absorption edge. A type-II heterostructure is formed at the interface of (F, Ti) codoped heptazine/triazine based g-C_3N_4 heterostructure, and leads to high photocatalytic activity. Furthermore, Bader charge and charge density difference indicate that the internal electric field promotes the separation of electron-hole pairs in the heptazine/triazine g-C_3N_4 interface and inhibits carrier recombination. Meanwhile, electrons in the conduction band of triazine g-C_3N_4 and holes in the valence band of (F, Ti) codoped heptazine g-C_3N_4 have enough redox ability. This work is helpful in understanding the mechanism of photocatalytic water splitting and relevant experimental observations.

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