Carbon, vol. 136: 187-195

Tuning the electronic structures, work functions, optical property and stability of bifunctional hybrid graphene oxide/V-doped $NaNbO_3$ type-II heterostructures: A promising photocatalyst for H_2 production

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ABSTRACT:

The depleting sources of nonerenewable fossil fuels and their adverse effect on the environment have driven the global interest to find an efficient and suitable material for hydrogen generation *via* a water splitting process. In this theoretical study, a bifunctional graphene oxide (GO)/V-doped $NaNbO_3$(100) heterostructure photocatalyst having a high stability and activity is studied for the first time using hybrid density functional theory calculations. The suitable type-II heterojunction structure between $NaNbO_3$(100) and GO sheet promoted the interfacial charge migration to restrain their recombination rate, thereby improving the activity of hydrogen generation. Moreover, the coupling GO sheet could offer conductive electron channels for the separation of electrons, hence further improve the photoresponse of $NaNbO_3$. The GO/V-doped $NaNbO_3$(100) heterostructure is a direct band gap semiconductor with a smaller effective mass compared with the pure $NaNbO_3$, which shows that the heterostructure has a higher charge carrier mobility. Thus, the resulting bifunctional GO/V-doped $NaNbO_3$(100) heterostructure is endowed with a suitable band alignment, narrow band gap, negatively charged O atoms on the $NaNbO_3$(100) surface and enhanced separation of charge carriers. This study offers new insights and valuable outlook to development of GO-based photocatalyst with visible light activity.