首届致远学术节
学生科研成果展示

Rose-like I-doped $Bi_2O_2CO_3$ microspheres with enhanced visible light response: DFT calculation, synthesis and photocatalytic performance

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Introduction

Over the past years, degradation of organic pollutants in effluents through photocatalytic processes has attracted much attentions. Bismuth based semiconductors have been widely developed because of their high photocatalytic activity. $Bi_2O_2CO_3$ is low mammalian toxicity for medicine treatment and shows high photocatalytic activity under UV light. However, the wide band gap of 3.0-3.5 eV would limit its utilization of solar light and photocatalytic efficiency. Therefore, we want to dope non-metal elements (like iodine) into photocatalysts to tune their band gap and we successfully synthesized rose-like I-doped $Bi_2O_2CO_3$ microspheres via a sodium citrate assistant hydrothermal process.

Key words

$Bi_2O_2CO_3$, Halogen doped, Cr (VI) reduction, Visible light photocatalysis

Results

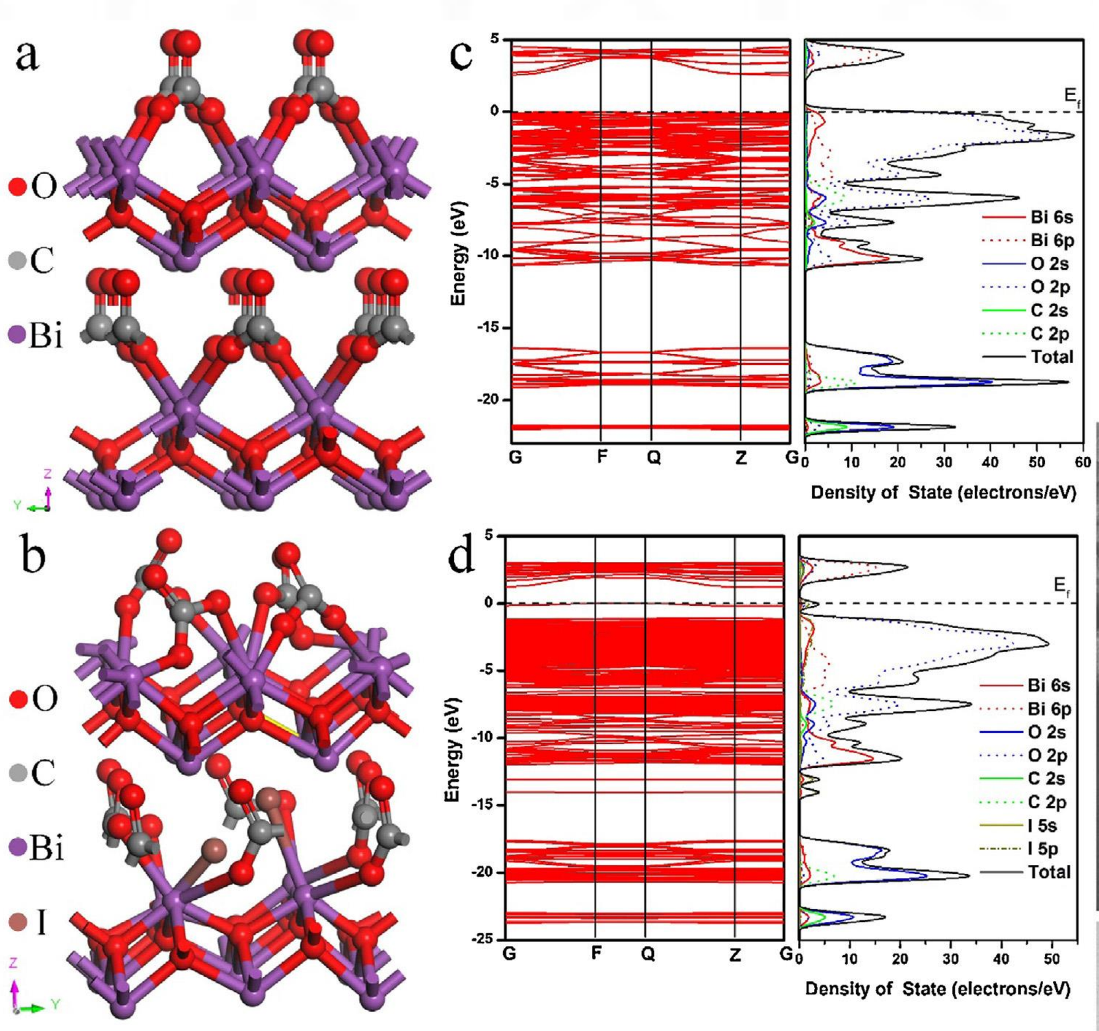

Fig. 1. Geometry optimized structure (a-b), band structures (c, d, right) and Density of state (c, d, left) of undoped (a, c) and I-doped (b, d) $Bi_2O_2CO_3$.

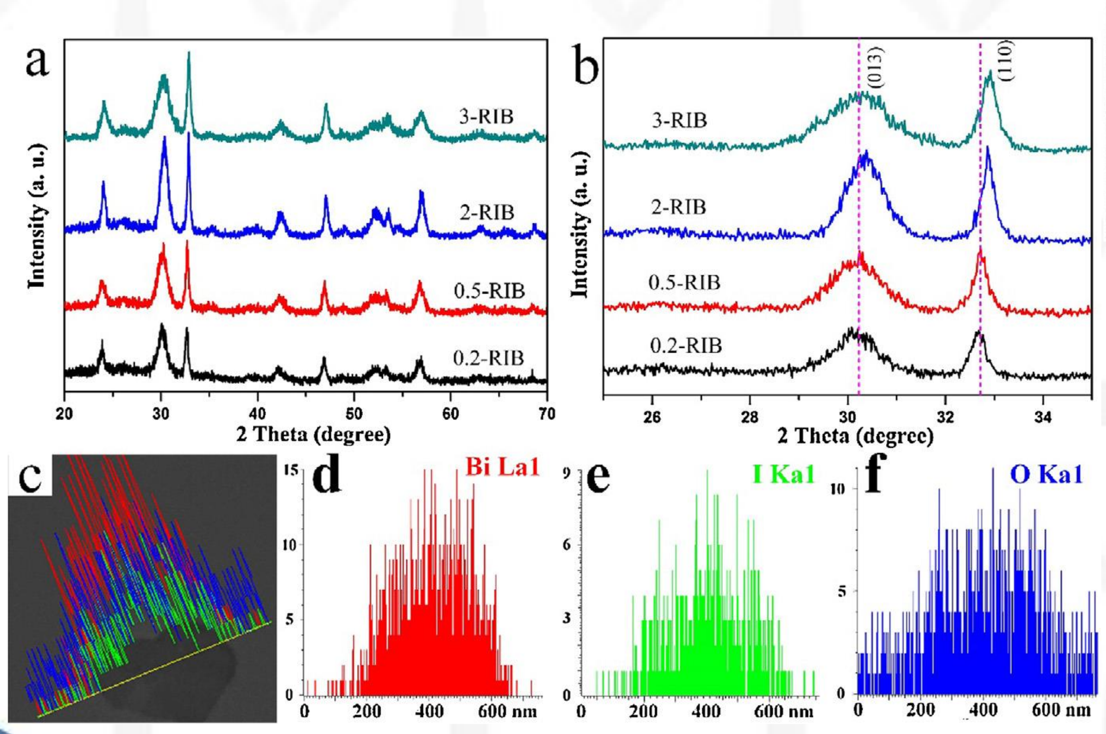

Fig. 2. (a) XRD patterns and (b) diffraction peaks of the (013) and (110) planes in the range from 25 to 35°of the obtained 0.2-RIB, 0.5-RIB, 2-RIB and 3-RIB; (c–f) EDS linear scan distribution map for Bi, I and O elements.

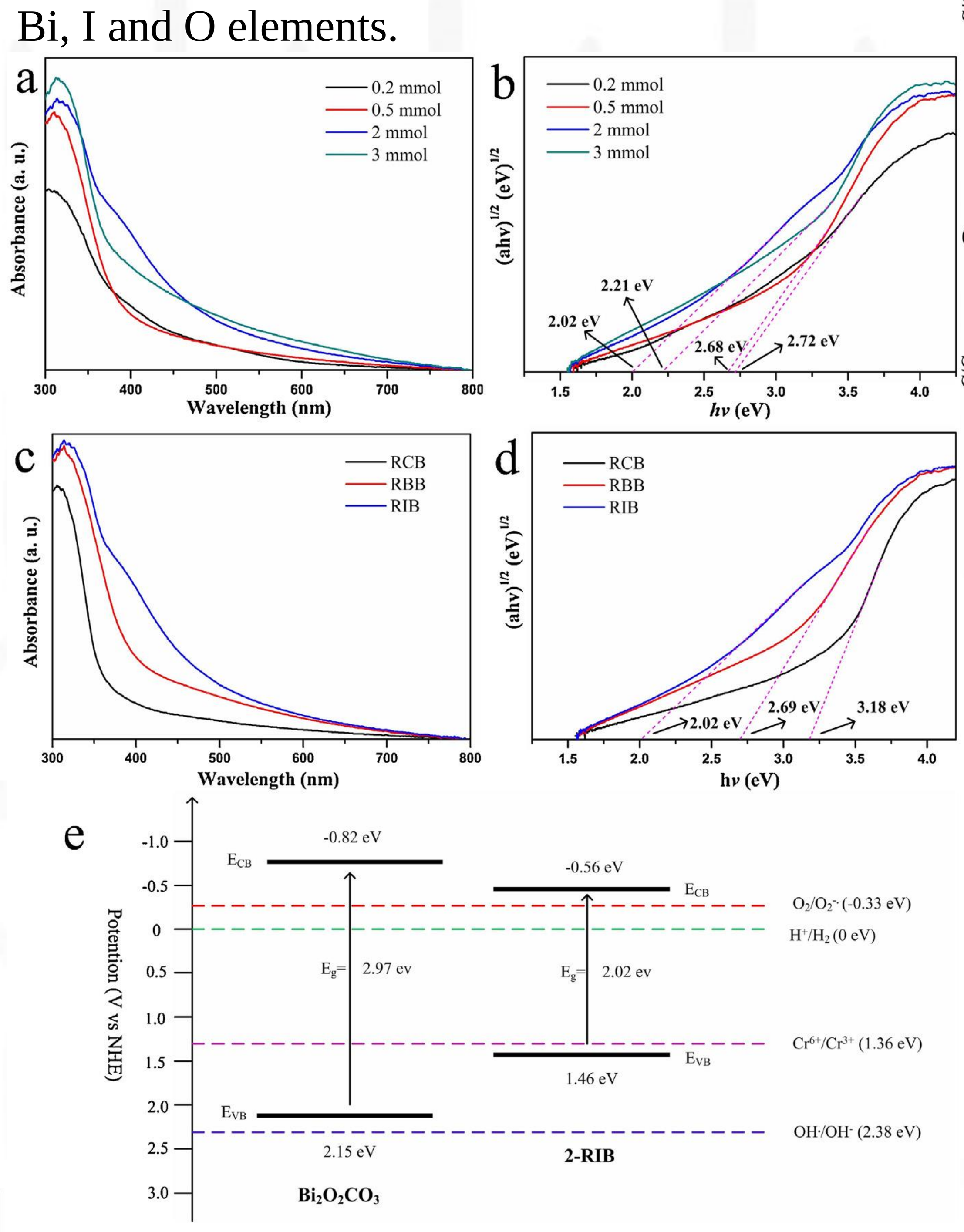

Fig. 3. UV–vis absorption spectra (a, c) and band-gap evaluation (b, d) from the plot of $(ahv)^{1/2}$ vs. hv of samples with different amount of I^-(a, b) and halogen elements (c,d). Band structure of 2-RIB and $Bi_2O_2CO_3$(e).

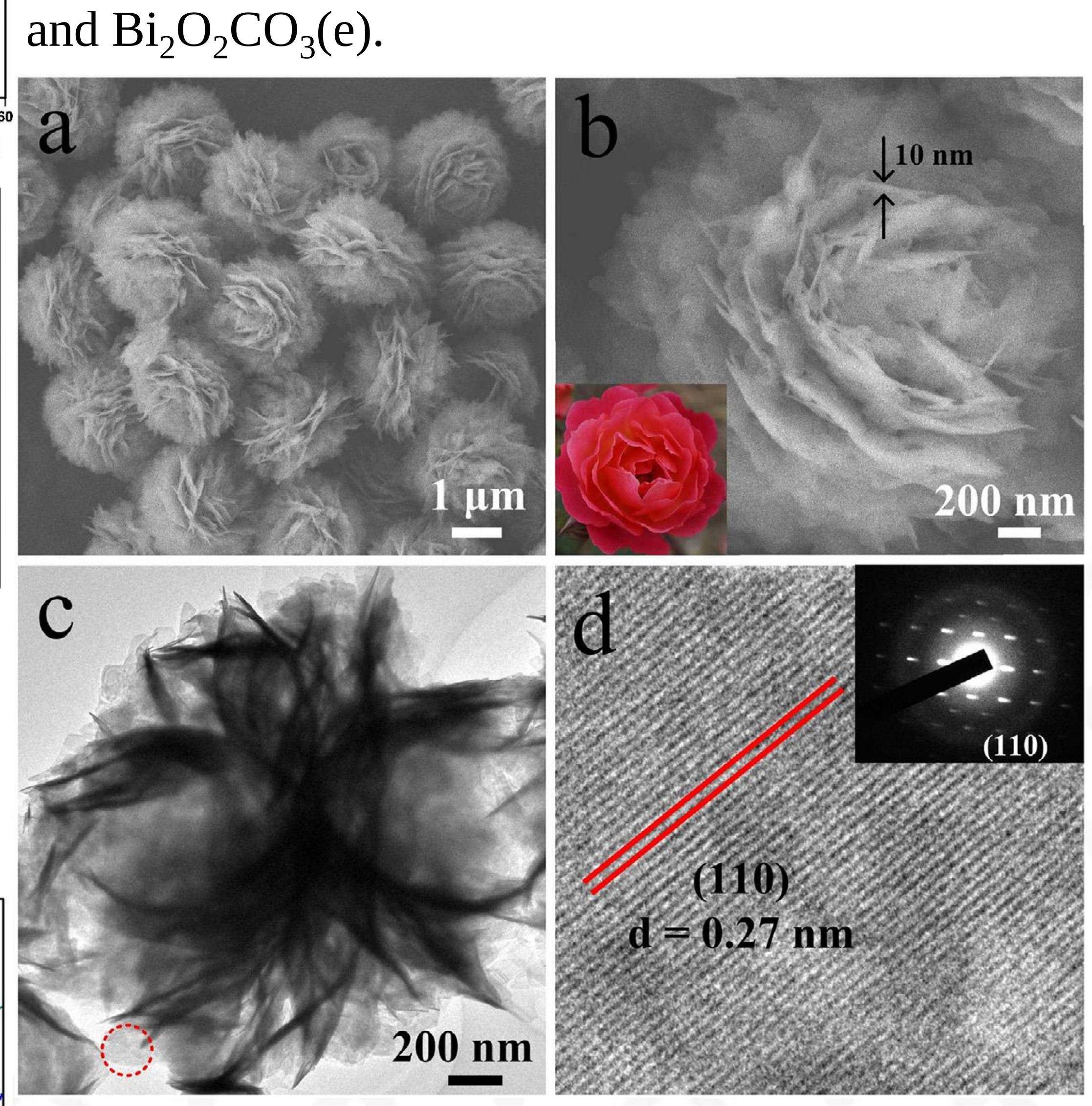

Fig. 4. (a-b) SEM, (c) TEM and (d) HRTEM images of 2-RIB. Inset of (d) is the corresponding SAED pattern.

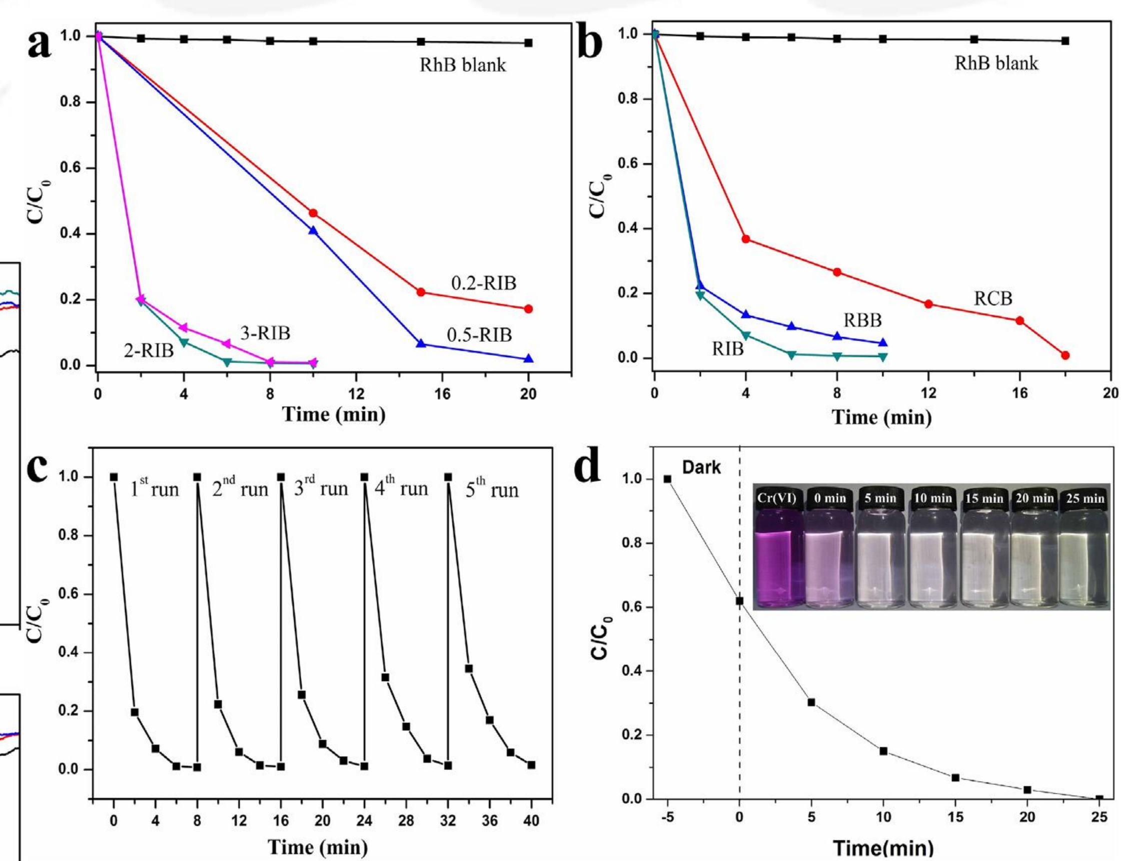

Fig. 5. Photocatalytic degradation of RhB using photocatalysts with different I amount (a) and halogen (b). Cycling of 2-RIB photocatalyst for degradation of RhB (c). Photocatalytic reduction of Cr(VI) with 2-RIB photocatalysts (d). All the photocatalytic experiments are under visible light irradiation (λ> 400 nm).

Conclusions

Rose-like I-doped $Bi_2O_2CO_3$ microspheres are prepared via a facile hydrothermal process. The photoresponse range of $Bi_2O_2CO_3$ can be tuned from UV to visible light by I-doping of different amount. The incorporation effects of I^- are verified by experiments and theoretical calculations. DFT calculation discloses that I^- can be doped into the crystal lattice of $Bi_2O_2CO_3$ by partial substituting CO_3^{2-}, and narrow the band gap of $Bi_2O_2CO_3$ by generating two intermediate levels in the forbidden band. The mechanism has also been confirmed by the good electrochemical performance. The as-prepared I-doped $Bi_2O_2CO_3$ photocatalysts exhibit excellent photocatalytic activity under visible light (λ> 400 nm) that RhB can be completely degraded within 6 min and all of Cr(VI)can be reduced after 25 min.

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