Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Synthesis and Structural Characterization of Novelty Visible Photocatalyst Bi-TiO_2/SBA-15 and Its Photocatalytic Performance

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Calculation model

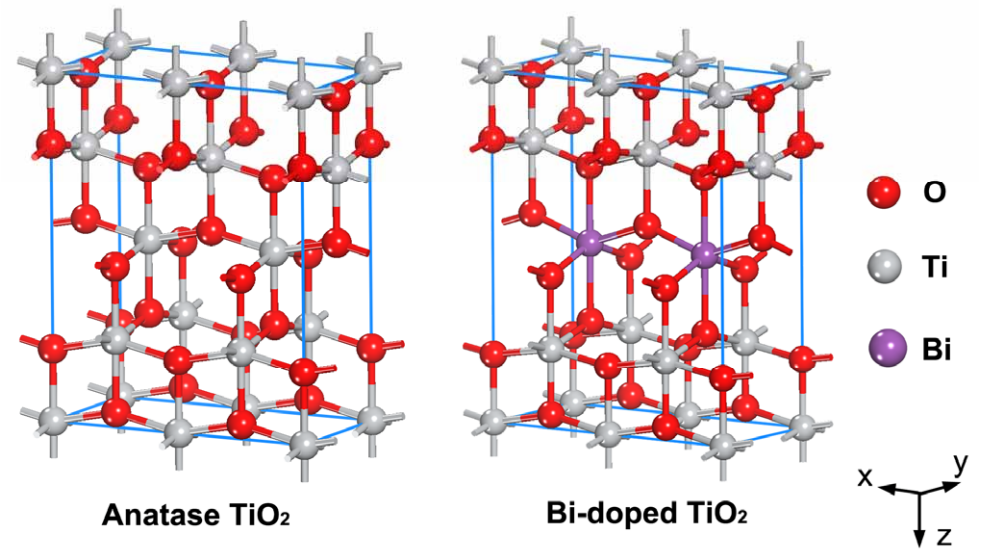

Fig.S1 Unit cell model of Anatase TiO_2 and Bi-doped TiO_2

The pure TiO_2 and Bi-TiO_2 systems were modeled using periodic boundary condition. Anatase TiO_2 has a tetragonal structure which contains two titanium atoms and four oxygen atoms in the unit cell. The anatase TiO_2 containing Bi atoms structure was labeled Bi-TiO_2 where the titanium atom was substituted for the bismuth atom.

Absorption experiment

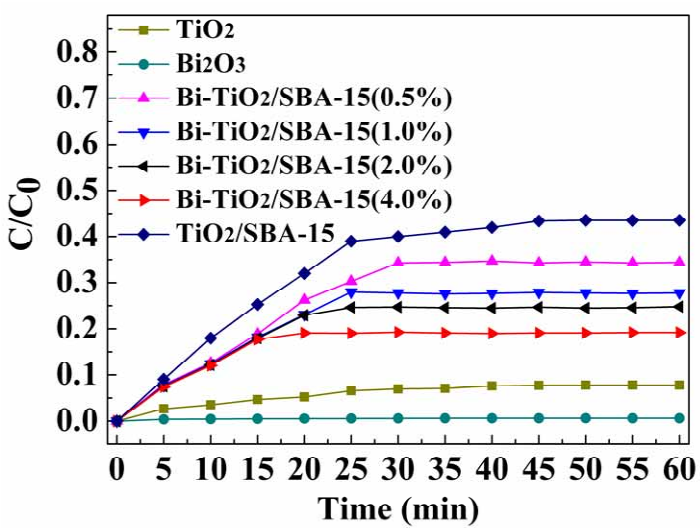

Fig.S2 Adsorption of RhB on Bi-TiO_2/SBA-15

Prior to irradiation, the suspension was stirred for 60 min in the dark in order to determine the time which allow a large contact between the RhB and the photocatalyst. At the initial stage, the absorption of RhB on the mesoporous Bi-TiO_2/SBA-15 material takes place. As absorption time proceeded, the absorption-desorption equilibrium between RhB and photocatalyst was established within 30 min and the absorption efficiency is ~20%, which indicated that the catalysts exhibited strong adsorption interaction with RhB.

Band structure of TiO_2

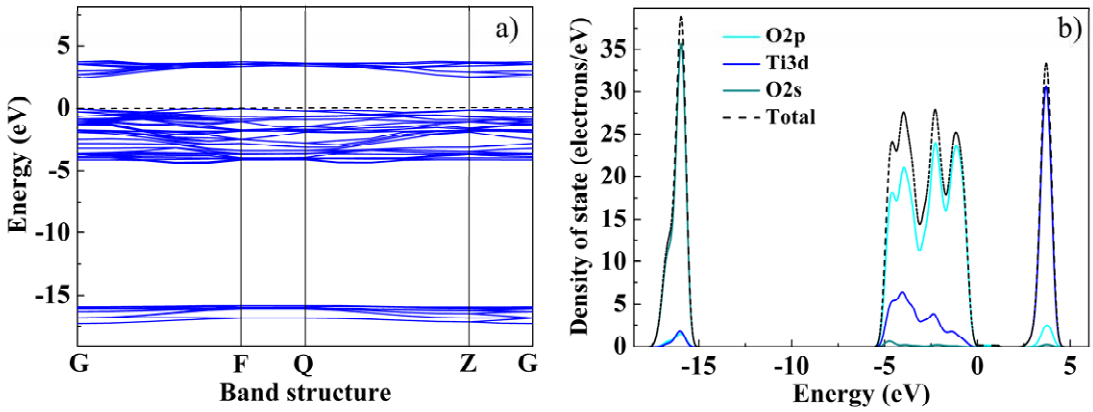

Fig.S3 Band structure a) and DOS b) for TiO_2 using the plane-wave DFT

The calculated band gap of TiO_2 is 2.47 eV, which is smaller than the experimental band gap 3.2 eV. This is in agreement with the precious observations [1]. It is worth nothing that this calculated band gap is smaller than the experimental result due to the inherent drawback of the ideal electron gas model in GGA approach [2].

[1] A. Heller, *Acc. Chem. Res.*, 1995, **28**, 503.
[2] T. Umebayashi, Y. Yamaki, H. Itoh and K. Asai, *Appl. Phys. Lett.,* 2002, **81**, 454.