Abstract Submitted
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Design of N-doped anatase TiO_2 photocatalyst with visible-light-response based on Ti-O bond weakening[1] L.-C. YIN, G. LIU, H.-M. CHENG, None, ADVANCED CARBON DIVISION TEAM — Nitrogen bulk doping is an effective strategy to change the electronic structures of anatase TiO_2 photocatalyst for visible light response improvement. Unfortunately, it is hard to achieve nitrogen bulk doping in practice, due to both limited thermodynamic solubility of substitutional nitrogen and N-induced recombination centers. It remains challenging yet highly desirable to develop new doping approach to increase nitrogen solubility in bulk. This challenge is originally stemmed from both strong Ti-O bond and charge difference (O^{2-} versus N^{3-}) between lattice oxygen and nitrogen dopant. In this work, we propose a new doping approach to promote the bulk substitution of lattice oxygen with nitrogen in bulk anatase TiO_2, based on the Ti-O bond weakening by pre-implanted interstitial boron.[1] By using the first-principles calculations, we study the interstitial boron induced Ti-O bonding weakening and the thermodynamics/kinetics changes for nitrogen bulk doping.[2] In experiment, we realize to synthesize a bulk gradient B-N co-doping red anatase TiO_2 microsphere which has an extended absorption edge up to ca. 700 nm covering the full visible light spectrum and has a bandgap varying from 1.94 eV on its surface to 3.22 eV in its core by gradually elevating VBM. This approach could be extended to modify other electronic materials that demand bulk substitutional doping. 1. G. Liu, J. Pan, L. C. Yin et al., Adv. Funct. Mater., 2012, 22, 3233. 2. G. Liu, L. C. Yin, J. Q. Wang et al., Energy Environ. Sci. 2012, 5, 9603.

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Teng Yang
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