

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Revisiting the mechanism of photocatalytic activities in N-doped TiO₂¹ NAOTO UMEZAWA, National Institute for Materials Science, JST PRESTO, JINHUA YE, National Institute for Materials Science, MANA — Photocatalysis possesses a great potential for environmental remediation and fuel production [1]. Nitrogen doped TiO₂ is a well-known visible-light sensitive photocatalyst where deep impurity states associated with substitutional nitrogen at oxygen sites (N_O) are believed to be the source of the red shift in photo-absorption edge. However, such a deep level should trap hole carriers, degrading oxidation process. The contradiction between the deep N_O level and rather a high oxidation power of N-doped TiO₂ has been an unsolved puzzle. Here, we propose a convincing mechanism which successfully solves the riddle. N_O strongly binds with a titanium atom at an interstitial site, forming a defect-impurity band, which consists of bonding and anti-bonding states of nitrogen p and titanium d and narrows the band gap. Such a newly formed band, which is connected to the valence band maximum of the host TiO₂, becomes the migration path of photo-induced hole carriers, assisting carrier transfer to the surface. This clearly explains the photocatalytic activity of N-doped TiO₂ both for the visible-light absorption and the oxidation reaction. [1] Hua Tong, Shuxin Ouyang, Yingpu Bi, Naoto Umezawa, Mitsutake Oshikiri, and Jinhua Ye, Advanced Materials DOI: 10.1002/adma.20110275

¹This work was supported by the JSPS KAKENHI (21760030) and the JST PRESTO program.

Naoto Umezawa
National Institute for Materials Science

Date submitted: 22 Nov 2011

Electronic form version 1.4