Joint CQSE and CASTS Seminar

Weekly Seminar
Mar. 29, 2013 (Friday)

TIME Mar. 29, 14:30 ~ 15:30

TITLE The Effect of Nitrogen-doping and Mechanical Strain on the Enhanced Visible Light Absorption of Anatase TiO_2

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Abstract

Atomic-level control and determination of the electronic band gaps of the semiconductor-based photocatalysts such as TiO_2 is of great importance for their applications in the challenging photo-electrochemical water splitting reactions using sunlight. Due to the relatively large band gap of TiO_2, only a small portion of the solar spectrum in the UV light region can be absorbed to excite electrons from the valence band top region to the conduction band edge of TiO_2 to generate photocurrents for use in photocatalytic reactions. Hence, many research efforts have been made to extend the absorption edge of TiO_2 to the visible light part of the solar spectrum to increase its photocatalytic efficiency under sunlight. Currently, one main strategy to achieve this goal is to dope TiO_2 with various transition metals or non-metal elements to effectively narrow down the electronic band gap of TiO_2. In particular, N-doped TiO_2 has recently become one of the most popular and widely investigated systems in the field of photocatalysis since Asahi *et al.*'s experiment in 2001. Nevertheless,the physical origins of the enhanced visible-light absorption of the N-doped TiO_2 remain unclear to date and many critical issues are still under intensive debate.

In the first part of today's talk, I will briefly introduce our recent work on studying the effect of nitrogen doping on the enhanced visible-light absorption of anatase TiO_2.Regarding this aspect, we have performed first principles calculations in conjunction with our newly developed method to investigate the long-term controversy regarding the effect of nitrogen doping on the electronic and optical properties of TiO_2. Our main focus here is to reveal whether the enhanced optical property is primarily attributed to the band gap narrowing of TiO_2 or that is simply induced by the excitation of the localized states within the electronic band gap. Moreover, we are also interested in finding out if there is

any other possible origin for the redshift-like behavior of the light absorption edge. In the second part of this talk, I will present our previous work on modulating the electronic properties of anatase TiO_2 via imposing auniaxial/biaxial mechanical strain. Based on first principles calculations, we have explored the effects of mechanical strains on the electronic band gap, VBM/CBM positions, and the effective masses of holes and electrons in anatase TiO_2. Our calculations showed that the effective masses of charge carriers and the band gap of TiO_2 can be effectively reduced by imposing mechanical strains along certain directions. This result also suggests that epitaxial growth of TiO_2 on some selected substrates/processing conditions could be a promising route toward enhancing the charge carrier mobility and the visible light absorption in anatase TiO_2.