Investigation of the effect of different particle size of N-doped TiO2 manipulated through controlled pH in sol-gel method on the band gap of the semiconductor and thus the photocatalytic ability of the material

Introduction

Research for the photocatalytic ability of TiO2 to decomposite water to yield hydrogen and oxygen at the presence of light is done in research years concerning human's increasingly urgent demand for developing an environmentally friendly method to produce renewable energy. The reaction was based on the semiconductor nature of TiO2. Electrons in the material have quantumized energy, and under photon simulation electrons could travel from their initial standard state to states with higher energy, which is called a migration from the valence band to the conduction band. Thus, an electron-electron hole is produced, which bear high reaction activity at the cost of short existence period. The h+/e- pairs which manage to migrate to the surface of the material without recombining could react with water through oxidation-reduction reactions, thus resulting in the decomposition of water.

However, it has been investigated that there's a preferred distance between the electron-hole pair calculated by the electro-static interaction between them, which is around 10nm. If given the premise that the particle size of TiO2 is less than the preferred distance, quantum sized effect would be initiated by limiting the production and movement of the e-/h+ pair. Thus, in this case, the migration of electrons from the valence band to the conduction band would possibly require more energy, meaning that the band gap (energy difference between VB and CB) would increase.

It's obvious that a higher band gap means a less proportion of photons with higher energy could initiate the formation of e-/h+ pair. Thus, only a smaller proportion of the sunlight with a more confined wave length range could be active. This could result in TiO2 particles with excessively s. mall particle size to bear a lower energy conversion efficiency.

On the other hand, the effect of surface area may imply a different trend between particle size and reaction efficiency. Since the reaction needs to take place on the surface of the semiconductor, higher surface area caused by smaller particle size could result in an increase of energy conversion efficiency. `

Proposed methodology

Researches have demonstrated the effect of pH in sol-gel method to synthesized nano-scale TiO2, which gives a general trend of increasing pH resulting in larger particle size. Particle size of TiO2 could be manipulated in experiments in this way. The particle sizes of samples would need to be checked through SEM microscope to obtain a precise data. The band gap of different samples could be obtained through the UV-Vis spectrometer.

With the obtained TiO2 particles, a set of equipment could be used to calculate the energy conversion efficiency. By placing the catalyst in a container which fully holds water under the presence of sunlight, and measure the output of gas during the reaction, a ratio between the input of sunlight radiation energy and the chemical energy obtained could be derived. By graphing the

relationship between the energy conversion efficiency and the particle size of TiO_2, an optimized value for particle size could be determined, which should expectedly appear around 10nm which ensures high surface area and small band gap.

Further innovation could be made based on the derived result and its explanation through the experiment. I personally expect to utilize the hydrogen yielded in a hydrogen fuel cell to produce electricity. In this way, by using the outputted electricity in certain items used in daily life like a coffee machine, a complete process of yielding and consuming renewable energy could be realized.