

# 5<sup>th</sup> International Conference on **Nanotek & Expo**

November 16-18, 2015 San Antonio, USA

## Theoretical investigation on heterogeneous photocatalytic systems containing metal oxide and aqueous solution

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To date, in the field of photo-catalysis using metal oxide inorganic materials, the most extensively studied systems have been the  $\text{TiO}_2$ -based materials. However, the efficiency in decomposing water molecule and producing oxygen and hydrogen upon sun light irradiation is still low. In an attempt at overcoming these limitations, photocatalytic properties of quite a few metal oxides different from  $\text{TiO}_2$  have been explored. Materials based on vanadate such as  $\text{BiVO}_4$ ,  $\text{InVO}_4$  and  $\text{YVO}_4$  were among them and might represent a promising alternative to  $\text{TiO}_2$ -based systems. Indeed, the  $\text{BiVO}_4$  can produce oxygen by photo-catalysis up to wavelengths of about 520 nm if the sacrificial reagent  $\text{AgNO}_3$  is added. However, no hydrogen generation has been reported to date. On the other hand,  $\text{InVO}_4$  shows hydrogen evolution in the visible wavelength range (from ultra violet (UV) to 600 nm) even from common liquid water, but it seems impossible to get oxygen. In case of the  $\text{YVO}_4$  system, it has been shown to possess surprisingly high efficiencies in both  $\text{O}_2$  and  $\text{H}_2$  productions in conjunction with the co-catalyst  $\text{NiO}_x$ . But the difficulty stems from its activity, which seems to be limited just to the UV region. The reason why these material systems indicate such contrastive photo catalytic properties was not cleared from a point of view of the electronic structure features on the bulk crystals of these materials, however, the electronic structures investigated by using inhomogeneous models including water and solid metal oxide photocatalysts equilibrated at room temperature obtained by applying first principles molecular dynamical simulations are now unraveling the mysteries. In this conference, I would like to introduce my research activities on metal oxide photocatalysts in this decade.

### Biography

Mitsutake Oshikiri received his PhD from Tokyo Institute of Technology (Japan) in 1992. He is now working in National Institute for Materials Science in Tsukuba, Japan. His main research activities are focused on the theoretical electronic structure properties on inhomogeneous systems and their applications in the field of photocatalytic reaction systems

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