World Journal of Engineering 7(4) (2010) 290-292

World Journal of
Engineering

Band gap of photo-catalyst slab system based on invo4 with water molecules adsorbed on the surface

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1. Introduction

It is known that $InNbO_4$, $InTaO_4$, and $InVO_4$ photo-catalysts indicate a visible light response in splitting water molecules (Zou *et al.*, 2001; Oshikiri *et al.*, 2002). Especially, the $InVO_4$ system has an outstanding feature that it can generate hydrogen from water up to the wavelength of approximately 600 nm although it cannot produce oxygen, while the other two can generate both hydrogen and oxygen but only up to the wavelength of approximately 500 nm. It seems that the component V atom plays an important roll to realize a good visible light response. However, it is also known that, for example, YVO_4 system shows a good performance in producing both hydrogen and oxygen but cannot indicate a visible light response at all (Ye *et al.*, 2003). What is the most interesting here is that only the $InVO_4$ can indicate an excellent visible light response in spite of the fact that the theoretically obtained band gaps of all these four bulk materials are almost the same (i.e. approximately 3.3~3.4eV). In an attempt at unraveling this issue, we have investigated the effect of the water molecule existence and its adsorption to the surfaces of the photo-catalysts $InVO_4$ and YVO_4, on the electronic structure properties of the systems equilibrated around at room temperature by first-principles molecular dynamics simulations using a super cell model.

2. Crystal structure properties

2. 1. YVO_4 crystal

In the YVO_4 crystal (a zircon-type crystal, the space group I4l/amd) (Baglio and Gashurov, 1968) each V is surrounded by four oxygen atoms forming a VO_4 tetrahedron (four-fold oxygen coordinated V; hereinafter called 4c-V) with an atomic distance of 1.71 Å between the V and the O, and each Y is surrounded by eight oxygen atoms forming YO_8 dodecahedron (8c-Y) with a Y-O distance of either 2.29 Å (for four of eight Y-O bonds) or 2.44 Å (for other Y-O bonds). The shortest V-V, Y-Y, O-O, and V-Y distances are about 3.9 Å, 3.9 Å, 2.6 Å and 3.1 Å, respectively. This YVO_4 crystal structure is characterized by the fact that every VO_4 tetrahedron is isolated by a YO_8 polyhedron. The conduction band minimum (CBM) of bulk YVO_4 is spanned by mainly V_3d atomic orbitals (~73 %), and the valence band maximum (VBM) is composed of O_2p (~83 %) (Oshikiri *et al.*, 2001)

2. 2. $InVO_4$ crystal

ISSN:1708-5284