Water molecule dynamics on a surface of InTaO$_4$ photo-catalyst

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The material InTaO$_4$ is known as a promising photo-catalyst which can produce both oxygen and hydrogen from water by visible light irradiation [1]. At this conference, detailed fundamental properties of InTaO$_4$ on the surface relaxation, water molecular dynamics and adsorptions on the surface, and some related electronic structures which have been investigated by first principles approach will be presented.

The surface structure relaxation and the water molecular dynamics on the surface were investigated by Car-Parrinello molecular dynamics simulation using a super cell ($\sim$ 250 Å$^2 \times$ 30 Å) including InTaO$_4$ slab ($\sim$10 Å thickness) with keeping a stoichiometric charge neutral condition. We prepared two kinds of slab surfaces. One exposes only four-fold oxygen coordinated Ta (4c-Ta) sites, and the other has 5c-Ta and 5c-In sites on the surfaces at an initial stage before relaxation although the bulk crystal is normally composed of TaO$_6$ (6c-Ta) and InO$_6$ (6c-In) octahedral structures. We investigated three cases: (1) without water, (2) with just a single water molecule, and (3) with bulk water. The thermodynamics was simulated by a velocity rescaling algorithm set at 300K for 1~2 pico-seconds.

Main results of this work are as follows; (1) Water molecules are easily dissociated at the 4c-Ta or 5c-Ta sites, however, they are often adsorbed undissociatively at the 5c-In sites. The water molecule adsorption energy at the Ta site is much larger than that at In site. (2) The band gaps of the slab systems with or without water are much smaller than that of the bulk crystal. (3) The O$_2$p orbital derived from water molecule which is disocciatively adsorbed to the surface is well mixed with the top of the valence band of the InTaO$_4$ photo-catalyst slab substrate although it is often mixed in the lower part of the valence band in other material systems (for example, see [2]).

We think that the fact that InTaO$_4$ system can produce both hydrogen and oxygen from pure water in visible light region should be deeply related to those results. This work might provide some good hints to pioneer new visible light response photo-catalysts able to generate both oxygen and hydrogen from water.