

Density functional theory based analysis of oxygen adsorption on anatase (001) surface^{o(D)}Nguyen Hoang Linh, Ganes Shukri, Hideaki Kasai

Department of Applied Physics, Graduate School of Engineering, Osaka University,

E-mail: kasai@dyn.ap.osaka-u.ac.jp

Studies of titania (TiO₂) have gained a lot of attention nowadays due to its various promising industrial applications such as gas sensors [1], organic dye-sensitized solar cells [2], solar energy conversion [3], etc. In almost applications of TiO₂, O₂ and H₂O are very important adsorbates which can significantly affect the redox processes on TiO₂ surfaces. However, while the process of water adsorption and dissociation on TiO₂ surfaces has been investigated for a long time [4, 5], there is still little knowledge about oxygen adsorption especially on reactive anatase surfaces. Along with the success in synthesizing the large percent of anatase crystal [6], the anatase surfaces nowadays are gaining interest especially in the surface chemistry field with its higher catalytic activity [7], particularly for obtaining full understanding of oxygen adsorption.

Anatase has two main available crystal facets: thermodynamically stable (101) surface and chemically reactive (001) surface. (001) surface was pointed out as an active surface for oxygen adsorption with lower energy adsorption [8]. Besides, it has been confirmed experimentally that nitrogen doping on TiO₂ surface increases oxygen vacancy formation and causes a substantial surface restructuring [9]. Therefore, it is necessary to investigate the N-doping effects on photocatalytic surface processes.

In this work, we focus on adsorption processes of oxygen molecule on anatase (001) surface by first-principles calculations based on density functional theory. The oxygen adsorption was systematically simulated on clean (001), O-poor (001) (with vacancy formation) and N-doped (001) surfaces. Adsorption characteristics (such as stable configuration, adsorption energy and electronic properties) as well as the influence of nitrogen doping on the oxygen molecule adsorption will be discussed.

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