Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Interfacial water on TiO_2 anatase (101) and (001) surfaces: First-principles study with TiO_2 slabs dipped in bulk water[1] YOSHITAKA TATEYAMA, MASATO SUMITA, International Centre for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), CHUNPING HU, Tokyo University of Science — Density functional molecular dynamics simulations using supercells with "bulk" water between the TiO_2 anatase (101) and (001) surfaces were carried out to elucidate the behaviour of water molecules and hydrogen bond networks on the interfaces of representative photocatalysts. It is demonstrated that the adsorption manners (molecular or dissociative) of water molecules on the vacuum surfaces still hold in the presence of "bulk" water on the interfaces. We also showed explicit atomistic structures of strong and weak hydrogen bonds on the TiO_2/water interfaces, which had been proposed experimentally so far. We then suggested a two-layer model for the interfacial water on both surfaces investigated. Our results also give insights into the H_2O or OH adsorption coverage on the interfaces and their hydrophobicity- hydrophilicity, which is important to understand the photocatalytic reaction mechanisms microscopically.

[1]This work wassupported by JST-PRESTO, JST-CREST and KAKENHI.

Yoshitaka Tateyama
International Centre for Materials Nanoarchitectonics (MANA),
National Institute for Materials Science (NIMS)

Date submitted: 30 Nov 2010 Electronic form version 1.4