

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Reaction path for dissociative water adsorption on vicinal anatase (101) surface¹ BERNARD DELLEY, Paul Scherrer Institut, ALFONSO BALDERESCHI, MICHEL POSTERNAK, EPF-Lausanne — Using density functional calculations and a periodical slab model, we investigate water adsorption on edges formed by intersection of two anatase TiO₂ (101) surfaces. We find that after adsorption of a water molecule on a low-coordinated Ti atom on the ridge, decomposition may happen over a moderately high barrier. In this process, a proton gets abstracted by bonding to a low-coordinated ridge oxygen atom. The hydroxyl anion remains bonded to the acidic Ti site on the edge. The methods used to find the saddle points and to map out the reaction paths are briefly discussed. We also give a discussion of the reaction rates that may be expected based on these calculations. The presence of hydroxyl groups and protons is favoring nucleation of Ca phosphate bonding by allowing exchange of the adsorbed proton against Ca²⁺ ions. Such processes are thought to be essential for the biocompatibility of titanium and its use in dental and orthopedic applications.

¹This work is supported by ITI Foundation for the promotion of Implantology, Switzerland.

Bernard Delley
Paul Scherrer Institut

Date submitted: 22 Nov 2008

Electronic form version 1.4