Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Structure and energetics of step edges on anatase TiO_2(101) XUEQING GONG, Princeton University, ANNABELLA SELLONI, Princeton University, MATTHIAS BATZILL, Tulane University, ULRIKE DIEBOLD, Tulane University, PRINCETON UNIVERSITY COLLABORATION, TULANE UNIVERSITY COLLABORATION — Defects, such as step edges, are of paramount importance to the physical and chemical properties of metal and metal oxide surfaces. However, while steps on metal surfaces have been extensively investigated both experimentally and theoretically, much less is known about the structure and properties of steps on metal oxide surfaces. Recent STM work examined the step structure of the (101) surface of anatase TiO_2 , which is the most stable and widely exposed surface of this interesting TiO_2 polymorph. Steps were found to exhibit a few preferred orientations, giving rise to islands with identical shape on the surface. Motivated by these observations, we have carried out extensive density functional theory calculations to determine the formation energies of steps along various orientations and with different structures. A procedure based on systematic calculations of related vicinal anatase TiO_2 surfaces has been used, which yields step edge energies with remarkable accuracy. The electronic structures of the stepped surfaces and adsorption of prototype molecules have been also investigated. The present results allow us to obtain a very detailed and complete understanding of the experimental observations.

Matthias Batzill
Tulane University

Date submitted: 30 Nov 2005 Electronic form version 1.4