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Adsorption of water on anatase TiO_2 nanoparticles: the role of a wire of undercoordinated Ti sites.[1] M. POSTERNAK, A. BALDERESCHI, EPF-Lausanne, Switzerland, B. DELLEY, Paul Scherrer Institut, Switzerland — Presence of hydroxyl groups is known to be an important element for the initial integration of titania–coated implants in natural tissues. The existence of OH^- radicals due to water dissociation is indeed responsible for major changes in their surface reactivity, and depends in particular on the preparation of the surface. The stable phase for nanoparticle–sized microstructures is anatase, and crystallites are expected to expose different surface terminations and edges. In this work, we study water adsorption on a model system, consisting of an edge along the $[1\,1\,\bar{1}]$ direction, at the intersection of two major (101) surfaces. Using the $DMol^3$ approach[2] within DFT, we find that water dissociative adsorption occurs at the four–fold coordinated Ti atoms present on this edge, in contrast with the case of the unreactive (101) surface. These results provide evidence of an increased chemical activity of such binding sites for adsorption of atoms and molecules. The mechanisms of the hydroxylation process are discussed in terms of the geometric arrangement, coordination numbers, and acidic/basic character of the relevant Ti and O sites.

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[2] B. Delley, J. Chem. Phys. **113**, 7756 (2000).

Michel A. Posternak
EPFL SB ITP CPNMC
PH D2 345, Station 3
CH-1015 Lausanne, Switzerland

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