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Structure of the rutile TiO_2(011)-(2x1) surface NAVID KHORSHIDI, ANDREAS STIERLE, VEDRAN VONK, CLAUS ELLINGER, HELMUT DOSCH, Max Planck Institute for Metals Research, Stuttgart, Germany, ULRIKE DIEBOLD, Tulane University, New Orleans, USA, XUEQING GONG, ANNABELLA SELLONI, Princeton University, Princeton, USA — TiO_2 has various applications in technology and is one of the most investigated metal oxides. It is used in solar cells and its photocatalytic activity makes an understanding of the structure of diverse surface orientations desirable. Although there are many studies on TiO_2 surfaces, the (011) surface has been rarely investigated. First principal DFT calculations predict the (011)-(1x1) face to have the third lowest energy and in a Wulff Construction a large part of the surface is (011) oriented. TiO_2 nano particles exhibit preferentially (011) oriented facets. Therefore a structure model of this surface is required to understand the photocatalytic processes on an atomic scale. We have investigated the TiO_2(011)-(2x1) surface using Surface X-Ray Diffraction (SXRD), Scanning Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED). From our data we are able to derive a novel model for the (011) surface in combination with DFT calculations. The new model has a much lower surface energy than the one suggested previously and fits the X-Ray data very well.

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