

Accepted Manuscript

Title: Novel (1×1)-reconstructions and native defects and of TiO_2 anatase (101) surface

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PII: S0169-4332(17)30403-8
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2017.02.052>
Reference: APSUSC 35161

To appear in: *APSUSC*

Received date: 30-11-2016
Revised date: 24-1-2017
Accepted date: 8-2-2017

Please cite this article as: Qinggao Wang, Fengzhu Ren, Huafeng Dong, Yuanxu Wang, Novel (1×1)-reconstructions and native defects and of TiO_2 anatase (101) surface, *Applied Surface Science* <http://dx.doi.org/10.1016/j.apsusc.2017.02.052>

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Novel (1×1)-reconstructions and native defects and of TiO₂ anatase (101) surface

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Highlights

- Acceptor energy levels are induced by O interstitials; corresponding to a transition of indirect-to-direct band gap and a narrowing of band gap. And thus, an experiment that the O-rich anatase TiO₂ has higher photocatalytic activity can be understood.
- The Fermi levels of defected and reconstructed TiO₂ anatase (101) can be modulated in a wide range (i.e., nearly the whole band gap), which are different from those of TiO₂ rutile (110).

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