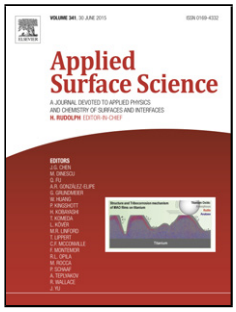

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Novel (1×1)-reconstructions and native defects and of TiO_2 anatase (101) surface

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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 TiO_2 has higher photocatalytic activity can be understood.
- The Fermi levels of defected and reconstructed TiO_2 anatse (101) can be modulated in a wide range (i.e., nearly the whole band gap), which are different from those of TiO_2 rutile (110).