

Abstract Submitted
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Coordination Defects and Nanoclusters of TiO_2 ¹ KEN PARK, Baylor University, VINCENT MEUNIER, MINGHU PAN, Oak Ridge National Laboratory, NAN-HSIN YU, Baylor University, WARD PLUMMER, Louisiana State University — Titanium oxide is one of the most investigated photocatalytic systems. It is capable of converting toxic organic and inorganic materials to benign products, as well as turning solar energy into a chemical one. Many believe that the catalytic activation involves charge transfer localized at surface defects with lower stoichiometry and/or coordination. In this study, scanning tunneling microscopy (STM) and density functional theory (DFT) are used to gain insight into such defects on $\text{TiO}_2(110)$. STM reveals defects ranging from a few Ångstroms to a few nanometers in size, but all of a uniform height of 3 Å. These topographically distinct defects are determined as fully stoichiometric nanoclusters by DFT. Despite the full stoichiometry, they possess undercoordinated atomic sites including 3- and 4-coordinated Ti and 1-coordinated O atoms. Their electronic and chemical properties will be discussed.

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