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TiO_2 Surface Defects with the Tetrahedral Cationic Coordination
KEN PARK, Department of Physics, Baylor University, VINCENT MEUNIER, Department of Physics, Applied Physics, & Astronomy, Rensselaer Polytechnic Institute, NAN HSIN YU, Department of Physics, Baylor University, WARD PLUMMER, Department of Physics & Astronomy, Louisiana State University — Titanium dioxide is one of the most extensively investigated transition metal oxide. It has well-known applications in catalytically converting toxic organic and inorganic materials to benign products, as well as turning solar energy into a chemical. In these processes, it is believed that surface defects with lower coordination and/or stoichiometry play crucial roles. Our study of a $(2\sqrt{2} \times \sqrt{2})$ R45 reconstructed $TiO_2(001)$ using scanning tunneling microscopy and density functional theory reveals that the basic building blocks of the reconstruction can be modeled as fully stoichiometric nanocluster defects. As in the bulk-terminated (001) surface, the atoms in the nanocluster are under-coordinated, for example, 4-coordinated Ti, 1-coordinated, and 2-coordinated O atoms. However, the absence of neighboring atoms drives the nanocluster to relax into a structure, which possesses tetrahedrally coordinated Ti atoms. This result will be compared and discussed with the reported nanocluster defects on $TiO_2(110)$.

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