

Abstract Submitted
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Electronic structure of N doped TiO₂: Hard x-ray photoemission study ABDUL RUMAIZ, National Synchrotron Light Source, Brookhaven National Laboratory, JOSEPH WOICIK, ERIC COCKAYNE, National Institute of Standards and Technology, HONG LIN, Dept of Materials Science and Engineering, University of Delaware, GHULAM JAFFARI, Dept. of Physics and Astronomy, University of Delaware, ISMAT SHAH, Dept of Materials Science and Engineering, University of Delaware — We have determined the electronic structure of N doped TiO₂ using a combination of synchrotron based hard x-ray photoemission spectroscopy (HAXPES) and first principle density functional theory calculations. Comparison with calculations and experiment reveals strong evidence of hybridization between different orbital components. Our results reveal that N doping of TiO₂ leads to the formation of oxygen vacancies and the combination of both N impurity and oxygen vacancies accounts for the observed visible light catalytic behavior of Ndoped TiO₂.

Abdul Rumaiz
Brookhaven National Laboratory

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