Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Bandgap Narrowing of Titanium Dioxides via Non-Compensated n-p Co-doping for Photocatalysis[1] WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory, BAOHUA GU, M. PARANS PARANTHAMAN, GYULA ERES, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory & University of Tennessee — Titanium dioxide (TiO_2) is a promising photocatalyst for solar hydrogen production from water, yet its photocatalytic efficiency is limited by its intrinsic wide-bandgap nature. In this talk, we present a conceptually new and intuitive approach, termed non-compensated n-p co-doping, to narrow the bandgap of TiO_2. The validity of this approach has been demonstrated using first-principles calculations within density functional theory, showing that extra impurity bands are created in the gap region because of the non-compensated nature of the n-p co-doping, resulting in a narrowed bandgap around 2 eV. Moreover, the electrostatic attraction between the n and p dopants enhances their thermodynamic and kinetic solubility in the host semiconductors. Preliminary experimental results confirming the non-compensated n-p co-doping concept will also be presented, together with its applicability to other wide bandgap semiconductors.

[1]Supported by the DMSE program and grant number DE-FG02-05ER46209 of US-DOE, grant number DMR-0606485 of USNSF, and LDRD program of ORNL.

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Date submitted: 29 Nov 2007 Electronic form version 1.4