Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Group IIIA doping in α-Fe_2O_3 for PEC hydrogen production MUHAMMAD N. HUDA, ARON WALSH, YANFA YAN, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, CO 80401, YONG-SHENG HU, ALAN KLEIMAN-SHWARSCTEIN, ERIC MCFARLAND, Dept. of Chemical Engineering, University of California at Santa Barbara, CA 93106, MOWAFAK AL-JASSIM, National Renewable Energy Laboratory, Golden, CO 80401 — Among iron oxides, α-Fe_2O_3 is the most abundant on earth. Because it has a band gap of approximately 2 eV, it is stable and inexpensive to process, α-Fe_2O_3 has been considered as a potential photoelectrocatalyst for solar driven photoelectrochemical (PEC) water splitting to make hydrogen. However, as α-Fe_2O_3 is a charge-transfer type insulator, the poor conduction properties have limited its efficiency as a PEC material. We will present our study on the doping of group IIIA elements in α-Fe_2O_3 to improve its performance. All the calculations were done with DFT+U. The main electronic features of α-Fe_2O_3 remained almost unchanged for group IIIA doping. While for Al-doping, the band gap remained almost the same, for Ga and In substitution the band gap marginally increased. However, increased conduction and PEC efficiency has been experimentally reported for Al-doped α-Fe_2O_3. It will be shown that the change in volume plays an important role in this behavior. A dramatic increase in photo-response cannot be expected for this type of doping in α-Fe_2O_3.

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Date submitted: 22 Nov 2008 Electronic form version 1.4