Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First-Principles Study of Photochemical Activation of CO_2 by Ti-based Oxides HAIYING HE, PETER ZAPOL, LARRY CURTISS, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439 — The photochemical conversion of CO_2 and H_2O into energy-bearing hydrocarbon fuels provides an attractive way of mitigating the green-house gas CO_2 and utilizing solar energy as a sustainable energy source. However, due to the high reduction potential and chemical inertness of CO_2 molecules, the conversion rate of CO_2 is impractically low. The activation of CO_2 is critical in facilitating further reactions. By carrying out first-principles calculations of reaction pathways from CO_2 to CO_2^- anions on Ti-based oxides including zeolites in the presence of photoexcited electrons, we have studied the initial step of CO_2 activation via 1e transfer. It is shown that the CO_2 reactivity of these surfaces strongly depends on the crystal structure, surface orientation, and presence of defects. This opens a new dimension in surface structure modification to enhance the CO_2 adsorption and reduction on semiconductor surfaces.

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Date submitted: 11 Nov 2012 Electronic form version 1.4