Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Computational Modeling of Photocatalysts for CO2 Conversion Applications DE NYAGO TAFEN, National Energy Technology Lab - URS Corp., 1450 Queen Ave. SW, Albany, OR 97321, CHRISTOPHER MATRANGA, National Energy Technology Lab, 626 Cochrans Mill Road, Pittsburgh, PA 15236 — To make photocatalytic conversion approaches efficient, economically practical, and industrially scalable, catalysts capable of utilizing visible and near infrared photons need to be developed. Recently, a series of CdSe and PbS quantum dot-sensitized TiO_2 heterostructures have been synthesized, characterized, and tested for reduction of CO_2 under visible light [1]. Following these experiments, we use density functional theory to model these heterostructured catalysts and investigate their CO_2 catalytic activity. In particular, we study the nature of the heterostructure interface, charge transport/electron transfer, active sites and the electronic structures of these materials. The results will be presented and compared to experiments. The improvement of our understanding of the properties of these materials will aid not only the development of more robust, visible light active photocatalysts for carbon management applications, but also the development of quantum dot-sensitized semiconductor solar cells with high efficiencies in solar-to-electrical energy conversion.

[1] C. Wang, R. L. Thompson, J. Baltrus, and C. Matranga. Phys. Chem. Lett. 2010, 1, 48; C. Wang, R. L. Thompson, P. Ohodnicki, J. Baltrus, and C. Matranga. J. Mater. Chem. 2011, 21, 13452.

De Nyago Tafen
National Energy Technology Lab - URS Corp.,
1450 Queen Ave. SW, Albany, OR 97321

Date submitted: 26 Nov 2012 Electronic form version 1.4