Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Thermodynamic Stability of Semiconductors for Photocatalytic Water Splitting[1] SHIYOU CHEN, LIN-WANG WANG, Lawrence Berkeley National Laboratory, MATERIALS SCIENCES DIVISION TEAM — Band structure engineering design of the light-absorbing semiconductors for water splitting has attracted wide attention recently. One of such design is to use the Z-scheme where a photocathode is connected with photoanode to reduce (generate H2) and oxidize (generate O2) water respectively. This requires the conduction band of photocathode and valence band of photoanode to straddle the redox levels of water. However, equally important in this design is the thermodynamic stability of the semiconductors in the aqueous solution upon illumination, i.e., the semiconductors may be oxidized (or reduced) before the water is oxidized (or reduced), causing the corrosion of the photoanode (photocathode). We will present our theoretical study on the thermodynamic stability of a series of photocatalytic semiconductors, including metal oxides, sulfides and nitrides, through the combination of phenomenological models for the semiconductor corrosion and the first-principles total energy and band alignment calculations. We find that almost all sulfides and nitrides are unstable as photoanode, while most of oxides are stable. This limits the choice of the photoanode materials for oxygen evolution. In contrast, for photocathode, most of the considered semiconductors are stable and resistant to reduction, indicating a much wider choice of the photocathode materials for hydrogen evolution.

[1]The work is supported by the Joint Center f Artificial Photosynthesis and the BES/SC of DOE under the contract No. DE-AC02-05CH11231, and the computation is performed using the NERSC and NCCS supercomputers.

Shiyou Chen
Lawrence Berkeley National Laboratory

Date submitted: 11 Nov 2011 Electronic form version 1.4