Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Optical Properties of GaN/ZnO solid solutions studied by Density Functional Calculations LI LI, P. B. ALLEN, State University of New York at Stony Brook — Semiconducting alloys of GaN/ZnO are promising hosts for solar photo-catalysis. The aqueous interface has been shown by Domen and collaborators[1] to catalyze water oxidation, a key half- reaction in water splitting. We calculate by DFT, the energetics of many $(GaN)_{1-x}(ZnO)_x$ supercell configurations. Results show that significant short-range order should be expected. A phase diagram is suggested from free energies calculated versus temperature and concentration. The mechanism of band gap bowing is examined. The DFT+U method and hybrid functionals are used to reduce the problems of band gap underestimation. Oscillator strengths near the band gap are calculated, and an ensemble-averaged dielectric function is constructed, with an aim to learn how to optimize solar light absorption.

[1]K. Maeda *et al.*, Nature **440**, 295 (2006).

Li Li
State University of New York at Stony Brook

Date submitted: 19 Nov 2009 Electronic form version 1.4