Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Water Adsorption on Wurtzite GaN Surfaces XIAO SHEN, PHILIP B. ALLEN, Stony Brook University, MARK S. HYBERTSEN, JAMES T. MUCKERMAN, Brookhaven National Laboratory — A solid solution of wurtzite GaN/ZnO absorbs light in the visible and can photosplit water.[1] The water is oxidized by the photo-holes at the surface of the semiconductor alloy. However, microscopic details of the oxidation process are unknown. We present a first-principles study of water adsorption on wurtzite GaN. We study the structures and energetics of water adsorption, calculate the energy barrier for water dissociation, analyze the water-water interactions, and study the electronic structure. The results are compared with water adsorption on ZnO surface. We also study the behavior of the holes near the water-semiconductor interface.

[1]K. Maeda, K. Teramura, D. Lu, T. Takata, N. Saito, Y. Inoue, and K. Domen, Nature 440, 295 (2006)

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Date submitted: 07 Jan 2009 Electronic form version 1.4