Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First principles study of the Ga(10$\bar{1}$0)/water interface[1] JUE WANG, XIAO SHEN, MARIVI FERNANDEZ-SERRA, Stony Brook University — Pure GaN is a water-splitting photocatalyst which works in UV light. A first-principles study shows monolayer of water molecules on the (10$\bar{1}$0) surface of wurtzite GaN have negligible barrier to be dissociated into OH^- which bind to Ga^+ and H^+ which bind to N^-.[2] We present an *ab initio* molecule dynamics study of bulk water molecules on top of the (10$\bar{1}$0) surface of GaN. The dissociation of water molecules happens very fast within the first ps of simulation. We find that $OH^- \cdot\cdot OH^-$ Hydrogen bond are formed between two OH^- on the surface. We propose two different types of OH^- based on the different H-bond structure between them and the bulk water molecules. We also calculate the vibrational spectrum and the interface electronic structure of the semiconductor/aqueous system.

[1]The work is supported by DOE grant DE-FG02-09ER16052
[2]X.Shen *et al.*, J. Phys. Chem. C **113**, 3365 (2009)

Jue Wang
Stony Brook University

Date submitted: 20 Nov 2009 Electronic form version 1.4