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First principles study of GaN(10$\underline{1}$0)/Water interface[1] JUE WANG, MARIA VICTORIA FERNANDEZ-SERRA, XIAO SHEN, Stony Brook University — GaN/ZnO alloy semiconductors have been shown to be promising materials to serve as photo-anode in photocatalytical fuel cells. In recent study by Shen et al[2], the non polar GaN(10$\underline{1}$0) surface has been studied with atomistic modeling and a sequence of intermediate steps for the water oxidation process at the interface are proposed. Here we present a first principles molecular dynamics study of the GaN(10$\underline{1}$0)/Water interface. We found dissociation events happen within 1ps and we show a detailed analysis of the changes in structure and dynamics of water molecules interacting with a dissociating wet surface. The complex hydrogen bond network near the surface is also analyzed in detail, including a throughout study of the proton diffusion processes. We perform a detailed analysis of the dynamics of the hole localization. The link between water surface dissociation and quantum efficiency will be discussed.

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[2]X. Shen, Y.A. Small, J. Wang, P.B. Allen, M.V. Fernandez-Serra, M.S. Hybertsen and J.T. Muckerman *J. Phys. Chem. C* **114(32)**, 13695 (2010)

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