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Water Oxidation on GaN Surface XIAO SHEN, JUE WANG, Stony Brook University, Y. A. SMALL, Brookhaven National Lab, P. B. ALLEN, M. V. FERNANDEZ-SERRA, Stony Brook University, M. S. HYBERTSEN, J. T. MUCKERMAN, Brookhaven National Lab — Efficient solar water-splitting requires a good catalyst to oxidize water into O_2 with the photo-holes. Efficient water oxidation catalysts are hard to find. The solid solution of wurtzite GaN/ZnO is a water-splitting photocatalyst which works in visible light, while pure GaN is a water-splitting photocatalyst which works in UV. Unlike other semiconductors, the surfaces of both materials exhibit high efficiencies for water oxidation. However, microscopic details of the reactions are not known. We present a first-principles study of water oxidation on the $(10\bar{1}0)$ surface of wurtzite GaN. The semiconductor/aqueous interface is modeled by a passivated $Ga_{15}N_{15}$ cluster, with two active sites (Ga atoms which bind OH^- ions, next to N atoms which bind H^+),[1] together with a few explicit water molecules and a polarizable continuum. We propose the key intermediates of a four-step mechanism for water oxidation on the GaN surface. We calculate the standard reduction potentials. The first of the four proton-coupled electron transfer reactions appears likely to be the rate-limiting step. We argue that our mechanism should likely apply to other semiconductor surfaces.

[1]X. Shen *et al.*, J. Phys. Chem. C **113**, 3365 (2009)

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