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Density functional study of GaN/ZnO alloy structure and surface properties[1] LI LI, XIAO SHEN, PHILIP B. ALLEN, Stony Brook University — Recent experiments[2] show that GaN/ZnO alloy is a promising host for photocatalytic water splitting. The band-gap of this alloy is narrowed down to the visible regime, allowing photo-absorption over a large portion of the solar spectrum. Muckerman et[3] made a first-principles studies of the structural and electronic properties of this alloy. We present further work on this alloy and on the surfaces which may host the water-splitting redox reactions. We look at structural properties such as bond lengths, and the stability of different configurations for various mixing ratios. We examine the nature of the HOMO and LUMO states, aiming for insight about the active sites of the water splitting catalytic chemistry.

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