

Abstract Submitted
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Band-gap bowing, band offsets, and electron affinities for AlN, GaN, InN and InGaN: A DFT study¹ POUL GEORG MOSES, CHRIS G. VAN DE WALLE, MAOSHENG MIAO, University of California Santa Barbara — AlN, GaN, and InN and their alloys are successfully being used in optical, electronic, and photovoltaic devices; a novel application is for photochemical water splitting. In order to further improve nitride-based devices a detailed understanding of the materials properties as a function of alloy composition is needed. To obtain such insight we have investigated the band gap and absolute band positions of AlN, GaN, InN and InGaN using density functional theory. The HSE exchange correlation functional has been used in order to accurately calculate the electronic band structure [1]. Detailed surface calculations have been performed that, combined with bulk calculations for alloys, yield information about the positions of valence and conduction bands on an absolute energy scale. We will discuss bowing effects, band offsets, and electron affinities in light of the application for photochemical hydrogen production.
[1] J. Heyd, G. E. Scuseria, and M. Ernzerhof, *J. Chem. Phys.* 118, 8207 (2003)

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