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Band-gap bowing, band offsets, and electron affinity for InGaN alloys: A DFT study.[1] POUL MOSES, CHRIS VAN DE WALLE, UCSB — InGaN alloys are successfully being used in optical, electronic, and photovoltaic devices; a novel application is for photochemical water splitting. In order to further improve InGaN-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 bowing and absolute band positions of InGaN alloys 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 of InGaN alloys for photochemical hydrogen production. [1] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003)

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