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Hybrid functional studies of InGaN alloys and oxides for photochemical watersplitting¹

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Photochemical watersplitting can potentially be a future sustainable energy source, converting sunlight and water into hydrogen. However, in order to have highly efficient devices materials are needed that absorb a large proportion of the solar spectrum while at the same time having valence and conduction bands that straddle the hydrogen and oxygen evolution redox potentials. It is well known that DFT consistently underestimates the band gap (the so-called “band-gap problem”). As a consequence, the positions of the valence and conduction bands (and hence the band offsets) also suffer from uncertainties. To address these deficiencies of the local density approximation (LDA) and generalized gradient approximation (GGA) we use the HSE exchange correlation functional in order to accurately calculate the electronic band structure [1]. We will discuss bowing effects in InGaN alloys based on accurate calculation of band gaps of InGaN alloys and on an analysis of experimental results using our calculated deformation potentials to disentangle the effect of strain and alloying on the band gap. We will also discuss calculations of the absolute position of the valence band maximum and the conduction band minimum. Including a discussion and comparison with generalized gradient and local density approximations results. Finally we show that HSE may be used to understand the nature of surface defects.

[1] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003)

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