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Band-gap bowing of InGaN alloys: A DFT study[1] POUL GEORG MOSES, QIMIN YAN, CHRIS G. VAN DE WALLE, University of California Santa Barbara — 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 of InGaN alloys and the strain effects in GaN and InN in the wurtzite phase using density functional theory. The HSE exchange correlation functional has been used 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 a analysis of experimental results using our calculated deformation potentials to disentangle the effect of strain and alloying on the band gap.

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

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